Doctoral Thesis

Electric transport phenomena in high mobility strained-Ge channels

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Electric Transport Phenomena in High Mobility Strained-Ge Channels

A dissertation submitted to the
SWISS FEDERAL INSTITUTE OF TECHNOLOGY (ETH) ZÜRICH

for the degree of
DOCTOR OF NATURAL SCIENCES

presented by
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2006
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Abstract

The traditional scaling approach to improving silicon based high performance electronics will encounter technological limits in the future. As a consequence, there is increasing interest in new materials with superior electronic properties. These materials are required to facilitate integration into existing production facilities. Chemically similar and available in sufficient quantity, germanium is one of the top candidates for follow-on technologies like Germanium-On-Insulator (GeOI). Strained germanium-on-insulator offers even higher performance, and can be manufactured by layer transfer or condensation techniques. Offering greater freedom of manufacturing conditions, layer transfer techniques require the strained film to be manufactured on a separate substrate, typically a silicon-germanium virtual substrate, and the properties of the film before transfer have direct impact on the final quality.

Investigation of the properties of Ge films embedded in the SiGe alloy provides the opportunity to study the fundamental properties of these films, in particular their electronic structure, i.e. their effective mass, and also their transport properties. Low temperature studies allow the identification of scattering mechanisms and interaction effects in the films. Apart from the usefulness for the application as a conventional semiconductor material, knowledge and improvement of the low-temperature mobility of the Ge films is needed for nanostructured devices like single-electron transistors or quantum point contacts that could be used in quantum computing.

Chapter 1 provides a more detailed introduction into present SiGe and Ge technology. The fundamental structural and electronic properties of silicon and germanium are reviewed.

Chapter 2 discusses sample and measurement details. The layer structure and the band offsets of Ge/SiGe heterostructures that lead to the formation of a 2-dimensional hole gas (2DHG) are discussed, and the fabrication of Hall bar structures is introduced, together with the electrical measurement setup. The important issue of sample heating by the measurement current and by external heating is discussed in detail. The principal ways of establishing thermal equilibrium between lattice and 2DHG are reviewed and estimates
are given to evaluate the relative importance of different equilibration paths.

Chapter 3 gives a detailed discussion of the in-plane band structure of the 2DHG and the quantization of energy in the growth direction of the sample. The band structure and the Landau level spectrum of the 2DHG are calculated. The band structure is used to calculate the density-of-states mass $m^*$ of the 2DHG under zero magnetic field conditions. This important material parameter is related to the effective mass deduced from Shubnikov–de Haas measurements in finite magnetic fields. The common assumption of the equality of density-of-states-mass and Shubnikov–de Haas mass is reviewed and shown to be violated above a 2DHG density of $1 \times 10^{12}$ cm$^{-2}$. At high carrier density, the effective mass found from Shubnikov–de Haas is significantly smaller than the density-of-states-mass. This is important since the Shubnikov–de Haas mass is frequently used to calculate zero-field properties, where the density-of-states-mass would be the appropriate quantity.

In chapter 4, the experimental dependence of the mobility of the 2DHG on the sheet carrier density is discussed. Samples with a mobility up to 120’000 cm$^2$/Vs and sheet carrier densities up to $8.5 \times 10^{11}$ cm$^{-2}$ were investigated. A theoretical calculation is performed for several scattering mechanisms and compared to the experimental values of the mobility, allowing to determine the dominating scattering mechanism. The impact on different doping geometries and growth related phenomena on sample properties are discussed. Predominance of interface charge scattering is found, while remote impurity scattering and charged background scattering are shown to be of only minor importance. In one case, short range scattering due to neutral defects is found to play a role as well.

Chapter 5 gives an overview over the magnetoresistive effects encountered in Ge/SiGe heterostructures at low temperature. Magnetoresistance related to band warping, weak localization and electron-electron interaction are discussed and compared to measurement results. It is shown that the combination of band warping and electron-electron interaction can explain the experimental observations. Band warping is responsible for the distinct positive magnetoresistance observed in the samples. The sheet carrier density dependence of the electron-electron interaction evidences the breakdown of screening as the carrier density is reduced.

Finally, the results are summarized and an outlook on the future potential of strained germanium and unresolved questions is given.
Zusammenfassung


Problem der Aufheizung der Probe durch den Messstrom und durch externe Wärmequellen wird im Einzelnen ausgeführt. Es werden die grundlegenden Arten besprochen, mit denen das thermische Gleichgewicht zwischen dem Kristallgitter und dem 2-dimensionalen Löchergas hergestellt wird und die relative Wichtigkeit der verschiedenen Wege zum Gleichgewicht wird abgeschätzt.


Im Kapitel 4 wird die Abhängigkeit der Mobilität des 2-dimensionalen Löchergases von der Ladungsträgerdichte diskutiert, wie sie im Experiment festgestellt wird. Proben mit einer Mobilität von bis zu $120'000$ cm$^2$/Vs bei einer Trägerdichte von $8.5 \times 10^{11}$ cm$^{-2}$ sind untersucht worden. Für verschiedene Streumechanismen wird eine theoretische Berechnung vorgenommen und mit den experimentellen Ergebnissen verglichen, wodurch die dominanten Streumechanismen festgestellt werden können. Die Auswirkungen verschiedener Dotierungsgeometrien und mit dem Probenwachstum zusammenhängende Phänomene auf die Probeneigenschaften werden diskutiert. Streuung durch geladene Grenzflächenzustände ist als dominanter Streumechanismus identifiziert worden, während Streuung durch die Dotierschicht oder durch homogen verteilte Ladungen nur von geringer Bedeutung sind. In einem Fall spielt auch Streuung durch neutrale Defekte eine Rolle.

Trägerdichteabhängigkeit der Elektron-Elektron-Wechselwirkung zeigt sich das Zusam-
menbrechen der Abschirmung beim Reduzieren der Trägerdichte.

Den Schluss bildet die Zusammenfassung der Ergebnisse und ein Ausblick auf das zukünftige
Potential verspannten Germaniums und die noch ungelösten Fragen.
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Dingle ratio</td>
</tr>
<tr>
<td>$k$</td>
<td>wave vector</td>
</tr>
<tr>
<td>$q, q$</td>
<td>scattering wave vector</td>
</tr>
<tr>
<td>$\chi$</td>
<td>density response function</td>
</tr>
<tr>
<td>$\epsilon_F$</td>
<td>Fermi energy</td>
</tr>
<tr>
<td>$\hbar$</td>
<td>reduced Planck’s constant</td>
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<tr>
<td>$\kappa$</td>
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<td>$\mathcal{E}$</td>
<td>electric field</td>
</tr>
<tr>
<td>$\mu$</td>
<td>mobility, chemical potential</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>wave function (chapters 3 and 4), digamma function (chapter 5)</td>
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<tr>
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<td>resistivity</td>
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<td>$\sigma$</td>
<td>conductivity</td>
</tr>
<tr>
<td>$\tau$</td>
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<td>transport scattering time</td>
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<tr>
<td>$\tau_q$</td>
<td>quantum scattering time</td>
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<tr>
<td>$\Theta(x)$</td>
<td>Unit step function</td>
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<td>$\varepsilon_r$</td>
<td>relative dielectric constant</td>
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<td>$D_u$</td>
<td>uniaxial strain matrix element (chapter 3)</td>
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<tr>
<td>$E$</td>
<td>energy</td>
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<td>Symbol</td>
<td>Definition</td>
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<td>--------</td>
<td>------------</td>
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<td>$e$</td>
<td>electron charge</td>
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<td>Fermi distribution function</td>
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<td>form factor</td>
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<td>$s_t$</td>
<td>transversal sound velocity</td>
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<td>temperature</td>
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<td>electrostatic potential</td>
</tr>
<tr>
<td>$v_F$</td>
<td>Fermi velocity</td>
</tr>
<tr>
<td>2-DHG, 2DHG</td>
<td>2-dimensional hole gas</td>
</tr>
<tr>
<td>CMOS</td>
<td>complementary metal-oxide-semiconductor device</td>
</tr>
<tr>
<td>CVD</td>
<td>Chemical Vapor Deposition</td>
</tr>
<tr>
<td>DOS</td>
<td>density of states</td>
</tr>
<tr>
<td>LEPECVD</td>
<td>Low Energy Plasma Enhanced Chemical Vapor Deposition</td>
</tr>
<tr>
<td>SdH</td>
<td>Shubnikov–de Haas oscillations</td>
</tr>
<tr>
<td>TEM</td>
<td>transmission electron microscopy</td>
</tr>
<tr>
<td>UV</td>
<td>ultra violet radiation</td>
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</table>
Chapter 1

Introduction

Today’s semiconductor market is dominated by silicon technology. In particular, the silicon CMOS technology is dominating most applications that do not require emission or absorption of light. Other semiconductor materials, such as the III-V compounds (e.g. GaAs, InP, etc.) have made their way into optoelectronics and into niche markets like high frequency applications.

For decades, the performance of electronics has followed Moore’s Law. This evolution was mainly driven by miniaturization, which allows both more and faster components to be integrated on a single chip. On the downside of this development were mainly increased power consumption and growing investment costs. Finally, it is easy to see that the process of reducing structure size is limited.

New materials offer the potential of cost savings if they can be integrated into existing production facilities (fabs). Integration onto a silicon substrate is required since it is the only crystalline material available in wafer sizes of up to 300 mm, which is the current production standard. In one way or the other, all proposed technologies rely on heterostructures to improve performance. These technologies include silicon-on-insulator (SOI, pretty much standard nowadays), strained silicon, strained silicon on insulator (SSOI), silicon-germanium on insulator (SiGeOI), to be combined with device technologies like double gate structures, high-k dielectrics and FinFETs. In the last case, the semiconductor is patterned into a thin stripe of high aspect ratio (like a fin, hence the name) and covered by the gate, which then acts from three sides instead of the top only, as in conventional technology, thereby improving performance.

Semiconductor heterostructures are structures made of different semiconductor materials.

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1Gordon E. Moore ( ∗ January 3, 1929), Co-founder of Intel corporation. Predicted the performance of computers to double every 12-24 months (sources vary)
The simplest type of heterostructure is a stack of different materials made by sequential deposition through a suitable process (this is called blanket deposition). Lateral structures are then typically introduced by photolithography. There are also processes by which the new material is deposited only at sites that have previously been patterned onto the substrate (selective deposition). Although attractive in principle, this method is still limited to certain materials and the substrate patterning required may be as involved as patterning a blanket after deposition.

1.1 Germanium for device applications

The use of silicon-germanium alloys started with the use of SiGe as base material \[^{1,2}\] in heterojunction bipolar transistors (HBTs) \[^{3}\], where the band offset between Si and SiGe is used to reduce the base-emitter drift current by orders of magnitude, permitting the use of a thinner base with higher doping, reducing the carrier transit time and increasing the maximum operating frequency of the transistor \[^{4}\]. Recently, operation at 500 GHz has been reported \[^{5}\].

Straining a silicon film by pseudomorphic deposition onto a relaxed SiGe layer improves electron mobility (see also section \[^{1,3}\]) parallel to the film. Extremely high operating frequencies can be obtained from n-type MODFET (Modulation Doped Field Effect Transistor) structures \[^{6}\]. There, conduction is mainly through a thin film of silicon, embedded in SiGe. The doping necessary to supply the carriers is only outside the channel, which improves carrier mobility because there are fewer scattering centers in the film. Today, this property is used extensively in mass production devices.

The lower mobility of holes compared to electrons in Si is a nuisance in device design for several reasons. For a given gate length, the switching delay is inversely proportional to the carrier mobility, making hole devices the speed limiter in CMOS (Complementary Metal-Oxide-Semiconductor) technology. This technology requires the use of a hole- and an electron transistor, driving the same output. The electron transistor is on when the input line has positive potential, and connects the output to ground. The hole transistor is on when the input line is grounded, and connects the supply voltage to the output, making the setup an inverter. Current only flows through the device when its state is switched, which is the great advantage, but at the cost of using hole devices. The lower mobility also leads to a lower value of transistor transconductance, requiring wider gates and bigger devices. Unfortunately, straining a Si film does little to alleviate the inferior performance of hole devices.

Due to its much higher hole mobility, germanium is considered as a future replacement of
silicon as far as device performance is concerned [7–15]. Amongst others, one challenge to date is the development of a suitable gate dielectric with high dielectric constant $k$. The mobility in such devices is higher than in similar Si devices [16, 17], but the high number of interface defects still limits it, sacrificing some of the intrinsic mobility advantage that Ge has over Si.

There is a strong interest in combining silicon and germanium technology to take advantage of the favorable properties of both materials. Silicon is lighter, stronger and cheaper than germanium, making it the material of choice for the structural support of electrical devices. Germanium, while offering superior mobility, suffers from its low resistivity at room temperature and above, which is due to its low bandgap. This leads to a high off-current, which increases power consumption. In addition, low resistivity makes it difficult to insulate devices, which can lead to crosstalk problems. One possible solution is to create a thin layer of germanium on an oxidized silicon wafer, for example by depositing a SiGe alloy and oxidizing it (condensation technique [18–20]) or by transferring an already formed thin Ge film onto the substrate [21–24]. Since the strain of the transferred layer is preserved, it is even possible to transfer a strained germanium layer onto the substrate, taking full advantage of the higher mobility.

Before transfer, strained Ge films are typically fabricated by lattice-matched (pseudomorphic) growth on a relaxed SiGe alloy, which allows to adjust the strain in the layer. The growth process has a large impact on the quality of the film. The properties of Ge films embedded in their host SiGe alloy are the subject of this work.

1.2 The silicon-germanium material system

For strained germanium to be transferred onto an oxidized silicon wafer, it has to be fabricated first. Pseudomorphic growth onto an unstrained SiGe alloys allows to adjust the strain as needed, since the lattice constant of the substrate can be tuned anywhere between the lattice constants of silicon and germanium, which possesses a 4% larger lattice constant than silicon. Pseudomorphic growth of SiGe alloys onto substrates of different alloy composition is thus always accompanied by the buildup of strain. Again, bulk SiGe wafers are not available, therefore the substrate is grown on a silicon wafer that serves as a template for single crystalline growth and provides the mechanical support. Several techniques exist to deposit a strain relaxed SiGe alloy on top of a silicon wafer. They differ in the way the strain of the SiGe layer is relaxed.

Strain relaxation through lattice defects is a plastic relaxation mechanism. Strain is relieved by eliminating lattice planes from the crystal, thereby increasing the average lattice
spacing. This gives rise to a lattice distortion along the boundary of the eliminated plane called a threading dislocation. Due to the energy associated with the formation of the lattice distortion, threading dislocations do not form immediately, but only when the strain is large or the activation energy for nucleation can be supplied by a nucleation site. After nucleation at the surface, threading dislocations move through the crystal. Ideally, the ends (“arms”) on the surface move until they reach the lateral boundary of the crystal, removing a complete plane. In reality, the arms get pinned before they reach the boundary, either by surface defects or by mutual interaction between individual threading dislocations, which is mediated by the strain field surrounding the dislocation core. As lattice imperfections, threading dislocations have a number of detrimental effects on electronic devices. Therefore, the quality of strain relaxed layers is generally judged by the number of threading dislocations needed to achieve a certain amount of strain relaxation, quantified by the area density of threading arms that penetrate the surface. As the counting techniques are either small area, offering bad or no statistics at all (plan-view TEM) or highly sensitive to external parameters (defect etching\textsuperscript{2}), comparisons between literature values are difficult.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>lattice constant $a$ [Å]</td>
<td>5.43095</td>
<td>5.64613</td>
</tr>
<tr>
<td>band gap $E_g$ [eV]</td>
<td>1.12</td>
<td>0.66</td>
</tr>
<tr>
<td>dielectric constant $\epsilon$</td>
<td>11.8</td>
<td>16</td>
</tr>
</tbody>
</table>

Table 1.1: Silicon and germanium fundamental properties

A germanium channel is typically grown in an environment of a relaxed SiGe alloy with a germanium content of 50–80%. Lower values of the Ge content of the SiGe alloy give higher confinement, but limit the maximum thickness of the Ge layer before plastic relaxation occurs. Silicon wafers are used as substrate, putting the emphasis on how to achieve relaxation of the layer directly underneath the channel with low dislocation density. This question was addressed in great detail by Meyerson, LeGoues and Tersoff of IBM\textsuperscript{[25–27]}. Their work and that of Fitzgerald, Xie and coworkers at Bell Labs\textsuperscript{[28–30]} showed that buffer layers with continuously graded germanium content give very long dislocation loops, i.e., the length of a threading dislocation is large. The threading arms of a dislocation can be separated by several centimeters, while the loop that joins them is injected down into

\textsuperscript{2}The etch should be too weak to attack perfect material, but strong enough to attack the disturbed crystal around a dislocation, requiring a different etch for each alloy composition. The resulting etch pits have to be counted. However, the pits are small and a certain (personal) bias is hard to avoid. Jokingly, this is sometimes commented on by the statement that good results were obtained by “doing the etch with deionized water and counting etch pits with closed eyes”.


the vicinity of the substrate, and sometimes even into it. This maximises the amount of relaxation for every dislocation that penetrates the electrically active layers close to the surface. Threading dislocation densities as low as $10^4$ cm$^{-2}$ have been reported, depending on the germanium content.

Ismail [31] showed how the density of threading dislocations influences the mobility. The dislocation density reduces with increasing buffer thickness (i.e. reducing grading rate). High mobility at liquid helium temperatures requires a grading rate below 10% per micron. The resulting buffer thicknesses of 10 µm or more pose a problem, however. The low thermal conductivity can lead to problems with cooling in high performance applications, and the high electrical conductivity impairs electrical device insulation. Fortunately, it is possible to transfer the strained layer to an oxidized silicon wafer, solving both problems simultaneously.

1.3 Electronic structure of strained layers

Strained layers offer an additional degree of freedom for device design. Since strain is a lattice distortion, it is possible to alter the symmetry properties of the strained layer. Application of biaxial strain to a (001) SiGe layer by enforcing a given lattice constant in two directions while not constraining the lattice in the remaining direction reduces the lattice symmetry from the cubic $O_h$ to the tetragonal $D_{4h}$ symmetry group. Degeneracies in the band structure are then partially lifted. The conduction band of silicon (6-fold degenerate band minima on the $\Delta$ line) is split into a 4-fold degenerate group and a two-fold degenerate pair. In the technologically important case of tensile strain, the latter is lower in energy and used in electrical transport. An additional benefit is the lower effective mass in transport direction. The conduction band of germanium is 8-fold degenerate with minima in the $L$-points. Their degeneracy is not lifted by this particular lattice distortion.

In contrast to the conduction band structure, the valence bands of relaxed SiGe alloys look very similar, irrespective of the alloy composition. The valence band can be viewed as formed from three identical atomic orbitals with p-character. Due to the spin-orbit interaction, one of them is lowered in energy and consequently called the spin-orbit hole band (SO-band). The remaining two bands are degenerate at the $\Gamma$ point, as shown in Fig. 1.1. Away from the $\Gamma$ point the degeneracy is lifted by the crystal field, leading to different dispersion relations with different effective masses. Therefore, the bands are called “heavy hole” (HH) and “light hole” (LH) band.
Chapter 1. INTRODUCTION

Fig. 1.1: The maxima of the hole bands in the band structure of bulk germanium are located at the Γ point \((k = 0)\), just below the Fermi energy (zero on the energy axis). They consist of the heavy holes (HH) and light holes (LH) (both indicated by \(\Gamma_8\)), and the spin orbit holes (SO, \(\Gamma_7\)). For \(k \neq 0\) the heavy and light hole degeneracy is lifted. Application of uniaxial strain lifts the degeneracy at the Γ point as well. Figure taken from [32]

The heavy hole-light hole degeneracy at the Γ point is lifted by the application of biaxial strain. In the above example, the heavy hole band is higher in energy when the biaxial strain is compressive, while tensile biaxial strain pulls up the light hole energy. Simultaneously, compressive biaxial strain decreases the effective mass of the heavy holes, increasing their mobility.

1.4 Scope of this work

The questions addressed in this work are the electronic structure of strained Ge quantum wells in relaxed SiGe claddings, the typical composition of which is Si\(_{0.3}\)Ge\(_{0.7}\). Electrical transport measured at temperatures below 20 K, where the channel properties can be obtained without interference from finite substrate conductance or the blurring effect of
1.4. SCOPE OF THIS WORK

phonons. A range of samples, grown on thick, strain relaxed buffers has been investigated for this purpose.

First of all, the band structure of the 2-dimensional states in the well is investigated by measuring the effective mass. This allows to compare experimental results to the results of band structure calculations. Agreement of measurement and calculation is crucial to ensure that band structure calculations for room temperature operation are reliable. Due to thermal occupation of multiple subbands, it is generally not possible to test the validity of the calculation at high temperature.

The mobility of the 2-dimensional hole gas at temperatures below 20 K is measured. In the absence of phonons, which are the dominating source of scattering at room temperature, the “built-in” scattering mechanisms can be determined from the dependence of the mobility on the sheet carrier density of the hole gas. To this end, a range of individual samples and several gated samples are investigated, and give a consistent picture of the sheet density vs. mobility dependence. Charged interface impurities have been identified as the main scattering source.

Finally, magnetoresistive effects are discussed which are induced by band structure, quantum mechanical interference and hole-hole interaction effects. The observed magnetoresistance is explained using the mentioned three mechanisms. The connection between the electron-electron interaction and the breakdown of screening on the way to the metal-insulator transition is highlighted. Future work on this aspect of the interaction effects is expected to yield interesting results.
Chapter 2

Experimental Setup

2.1 Sample structure

An schematic of the sample structure is shown in Fig. 2.1. A detailed description of the LEPECVD deposition system is given in appendix B. Directly on top of a commercial Si (001) wafer, a virtual substrate is deposited. It consists of a buffer layer in which the Ge fraction is graded at 7% / µm up to a final concentration of 70% Ge and a 2 µm thick constant composition part which reduces the strain fields associated with the relaxation in the buffer.

The electrical structure consists of the lower cladding of 50–100 nm Si$_{0.3}$Ge$_{0.7}$, the 10–20 nm germanium channel, the upper cladding with the same composition as the lower one, the remote doping layer, a cover layer with the same composition as the cladding and a 2-3 nm thick silicon layer which protects the lower layers from oxidation.

Small samples for electrical characterization can simply be cleaved from the wafer after scribing the backside with a diamond tip. The sample shape is trivial to control in this way. The method of van der Pauw [33] has to be used to determine the resistivity. For the van der Pauw technique magnetoconductivity measurements require multiple sweeps to measure the resistivity and the Hall effect. These measurements become more convenient when samples are patterned into the form of Hall bars (Fig. 2.2), albeit at the expense of additional processing.

The shape is etched into the layer stack by chemical wet etching and metallic contacts are formed by conventional lift-off techniques. For a detailed description of the fabrication process see appendix C. Hall bars allow simultaneous measurement of the resistivity and the Hall effect in a single magnetic field sweep and give a very symmetric magnetoresistance. The only shortcoming of the Hall bars used is that the cladding has a rather
Fig. 2.1: The typical layer structure of the samples comprises a virtual substrate to adjust the strain of the channel and the cladding around the channel which serves as a barrier to the carriers that are confined to the channel. The cladding composition may differ from that of the virtual substrate. One or several doped layers (blue) in the cladding supply holes (green) to the channel. While the virtual substrate requires high growth rates, the active stack is deposited slowly to allow precise thickness control. Due to the unique ability of the LEPECVD system to adjust the growth conditions (see appendix B), the complete stack can be grown without interruption in a little more than one hour. The thicknesses of individual layers given on the left can vary from sample to sample, and the doping may be underneath the channel as well as above.

Fig. 2.2: From the layer stack, Hall bars are fabricated by etching through upper cladding (blue) and channel (red) into the lower cladding (blue). Parts that are not etched are called “mesa”. The contact pads (yellow) are then covered with metal and annealed to form ohmic contacts.
high conductivity at room temperature. Conduction through the lower, unetched layers is dominant down to about 100 K and prevents measurement of the channel properties at higher temperature.

2.2 Electrical setup

Electrical transport measurements of the 2-dimensional layers were performed using a Quantum Design Physical Property Measurement System (PPMS). The accessible temperatures of this cryostat range from 1.9 to 300 K and the magnetic field can reach values up to 14 T. When a special $^3$He insert is used, the temperature can be lowered to 0.5 K in continuous operation and to 0.3 K for a limited time (1-2 hours, depending on the initial amount of liquid $^3$He).

The current is forced through the sample by a constant current source (see Fig. 2.3). This source consists of a constant voltage source provided by a Stanford Research 830 lock-in amplifier, a Lundahl LL 1540 high impedance input transformer and two 5.1 MΩ resistors. Because the resistors have a much higher resistance than the sample, the current is independent of the sample resistance. The task of the transformer is to remove connections to ground. Thus the ground connection can be chosen as desired or left open.

The SR 830 that produces the excitation voltage also generates a synchronization signal used for phase sensitive detection of the voltage appearing on the voltage terminals of the sample.

If the sample is equipped with a gate electrode, a gate bias can be applied between the gate electrode and the middle of the secondary coil of the transformer. Therefore the gate voltage is symmetric with respect to the current terminals. This means that the gate voltage does not change during a cycle of the excitation current. The 5.1 MΩ resistors also provide protection to the gate structure in case of a gate breakdown by limiting the current, which could otherwise lead to a destruction of the sample. The gate voltage is usually supplied by a battery driven voltage divider which is adjusted manually. This has the advantage of not introducing noise into the measurement, but it suffers from limited battery lifetime and it cannot be automated.

When Hall bars are used, the resistance is measured simply by forcing current along the bar and measuring the voltage difference of two adjacent voltage probes (connected to LIA 1 in Fig. 2.3). The resistivity can then be calculated by dividing the measured resistance by the aspect ratio of the Hall bar between the probes. In our case, this aspect ratio is 5. For square shaped samples, the method of van der Pauw [33] is used.
Fig. 2.3: Measurement setup for magnetotransport measurements. The excitation voltage from the upper Lock-in amplifier (LIA) is fed into the sample (blue) via a transformer and two symmetric $5.1\,\Omega$ resistors, giving a constant excitation current. The second LIA is phase locked to the excitation by a TTL synchronization signal. The gate voltage $U_G$ is referenced to the symmetric tapping of the transformer secondary, so that the gate voltage does not change during the duration of an excitation cycle. Typically, the gate (red) is driven by a battery-powered voltage divider to reduce noise.

### 2.3 The temperature of the hole gas

Quantum corrections to the classical (Drude) conductivity of 2-dimensional systems generally show a logarithmic temperature dependence. The temperature at which they become measurable is usually only a few Kelvin, sometimes even below one Kelvin. The temperature dependence of scattering times, e.g., in weak localization, is used to identify the type of scattering. Therefore it is crucial to precisely determine the temperature of the hole gas. As will be shown, this temperature is not necessarily identical to the cryostat base temperature. The question whether the temperature of the hole gas is what it appears to be will become relevant in chapter 5. In the case of Si/Si$_{0.8}$Ge$_{0.2}$, the hole energy relaxation
has been studied in detail \[34, 35\].

Ohmic heating of the 2-dimensional hole gas is a direct consequence of passing a current through the sample to measure its transport properties. If this heat is not removed at a sufficient rate, the temperature of the gas can be considerably higher than the temperature of the heat reservoir. In general, the bottleneck for heat flow in the experiment is the heat transfer from the hole gas to the phonon gas in the lattice of the sample. This transfer can be effected both directly by emission of phonons and indirectly by flowing the heat into the electron gas of the contact metalization.

Both processes work well at high temperatures. As the temperature is decreased, heat transfer becomes slower. The fact that for a given heating power there is a minimum temperature that can be achieved has severe consequences. In particular, an independent method of determining the temperature of the carrier gas is needed. The simplest test to recognize heating effects is of course to change the current through the sample. Unfortunately, the observation that there is no significant change in the measurement does not exclude electron heating if the source of heating is due to other sources than the measurement current itself, for example by capacitively or inductively coupled currents in the sample. The heat dissipated by an external heat source can be estimated by measuring the minimum measurement current required to significantly heat the sample. The external heat source has a power similar to that of this current.

### 2.3.1 Phonon cooling

Phonon emission leads to homogeneous cooling of the carrier gas. The cooling power scales with sample area and depends on the temperature. If the conditions \( T \ll \hbar c/w k_B \) and \( T \ll \sqrt{2m_F c/k_B} \) are fulfilled, the cooling power behaves like \( P \propto T_e^5 - T_{\text{bath}}^5 \). The first condition requires the wavelength of a typical phonon to exceed the well width \( w \), while the second requires the Fermi momentum to be much larger than the momentum of an average phonon. Under these circumstances, the power loss per carrier from the carrier gas to the phonon gas is given by \[36, 37\]

\[
P = \frac{3\zeta(5)D_u^2k_B^5(2m^*)^{1/2}}{\pi\rho_M\hbar^4s_t^4\epsilon_F^{3/2}} \left[ D^2 + D + \frac{3}{8} + \frac{1}{8} \left( \frac{s_t}{s_l} \right)^4 \right] (T_e^5 - T_{\text{ph}}^5) \tag{2.1}
\]

where \( \zeta(5) \approx 1.04 \), \( D_d = 12.7 \text{ eV} \) is the deformation potential for hydrostatic strain, \( D_u = 3.9 \text{ eV} \) is the deformation potential for uniaxial strain, \( D = D_d/D_u = 3.25 \), \( \rho_M = 5323 \text{ kgm}^{-3} \) is the mass density and \( s_l = 4900 \text{ ms}^{-1} \) and \( s_t = 3500 \text{ ms}^{-1} \) are the longitudinal and transversal sound velocities. For typical Ge samples, the prefactor
(in front of the square brackets) evaluates to about $10^{-17}$ W/K$^5$, which will be used in the following. To get the total cooling power, one has to multiply this prefactor with the number of carriers in the sample, making large samples easier to cool. The $T^5$-dependence leads to a rather abrupt decoupling of electrons and phonons below a certain phonon temperature. Calculated and measured data by Braithwaite et al. [35] give a value of $P = 8 \times 10^{-18}$ W/K$^5$ for Si/Si$_{0.2}$Ge$_{0.8}$, independent of the carrier density which ranged from $3.0 \times 10^{11}$ cm$^{-2}$ to $7.7 \times 10^{11}$ cm$^{-2}$ in their experiment, while Xie et al. [34] give a value of $4.6 \times 10^{-18}$ W/K$^5$. The latter group claimed additional contributions from piezoelectric scattering, which explains the lower value for deformation potential scattering. Values for pure Ge are not readily available, but given the similarity of the relevant quantities, the value of $10^{-17}$ W/K$^5$ calculated above seems realistic.

For example consider a sample with sheet resistance $\rho = 250$ Ω, and carrier density $p_s = 4.5 \times 10^{11}$ cm$^{-2}$, patterned into a standard Hall bar 750 µm long and 50 µm wide. The total number of carriers in the sample is $1.69 \times 10^8$, the cooling power is approximately $2.4 \times 10^{-9}$ W/K$^5$. When a current of 400 nA is forced, the electron temperature $T_e$ will never drop below 0.76 K, even if $T_{ph} = 0$. However, if $T_{ph} = 1.00$ K, the electron temperature is 1.04 K, which can be tolerated in most experiments. With the lowest possible measurement current of 10 nA and a phonon temperature of 0.3 K, the electron temperature would be 0.303 K, and heating effects would hardly be detectable in experiment.

### 2.3.2 Diffusive cooling

Carrier diffusion into the contacts lets the heat flow away in a 2–D heat flow. The metalized contacts form the heat reservoirs. Similar to electrical conduction, the dimensionality of the system leads to a heat conductivity independent of the sample size, only depending on its shape. Interestingly enough, simulations show that the part of the Hall bar that is usually used to measure the resistance of the sample is the area that heats up the most under these circumstances. As the thermal conductivity $\kappa$ of a Fermi gas is proportional to $T$ and the electrical conductivity $\sigma$ (Wiedemann-Frantz-Law), low mobility samples should be affected more than high mobility samples:

$$\kappa = \frac{\pi^2}{3} \left( \frac{k_B}{e} \right)^2 \sigma T \quad (2.2)$$

For example, with $T = 1.00$ K and $\rho = 250$ Ω we get $\kappa = 9.8 \times 10^{-11}$ W/K. The total power dissipation in a strip with 15:1 aspect ratio and a current of $i = 400$ nA
2.3. THE TEMPERATURE OF THE HOLE GAS

is \( P = 15 \times 250 \times 1.6 \times 10^{-13} \text{ W} = 6.0 \times 10^{-10} \text{ W} \), the thermal conductivity is about \( 10^{-10} \text{ W/K} \) so that there would be a strong temperature increase.

\[ T_{\text{lattice}} = 0.35 \text{ K} \]

**Fig. 2.4:** Calculated decoupling of hole gas temperature and lattice (phonon) temperature, taking into account phonon and diffusive cooling. Red symbols show peak temperature, blue symbols average temperature. The example parameters are chosen to reflect those of sample 7404-16 (see section 5.2.4), a Hall bar. It has a length \( l = 750 \mu\text{m} \), width \( w = 50 \mu\text{m} \), resistivity \( \rho = 250 \Omega \), and carrier density \( p_s = 4.5 \times 10^{11} \text{ cm}^{-2} \). At a sample current of 100 nA (upper right, used most frequently), the gas temperature follows the lattice temperature down to about 0.7 K. At lower temperature, the gas is significantly hotter than the lattice. As the current is reduced to 20 nA (lower left), lattice and gas have equal temperature down to 0.35 K, the lowest temperature possible in the cryostat used. At 400 nA, the sample cannot be cooled below 0.8 K (upper right).

Depending on their aspect ratio, the voltage leads are able to remove a lot of heat from a Hall bar. While usually thinner than the current leads, they are also shorter, and they do not contain any heat sources.

In **Fig. 2.4**, a calculation for sample 7404-16 is shown. The model takes into account phonon cooling (2.1) and diffusive cooling (2.2) and uses a finite element calculation to
model the heat flow through the Hall bar. Under these circumstances, most of the heat is removed by phonon emission. Only in the parts of the Hall bar close to the contacts, significant heat is removed into the metalization by 2-dimensional heat flow. At temperatures above $\sim 1$ K, the hole gas temperature agrees with the lattice temperature for all measurement currents used (up to 400 nA). As the temperature is reduced, the hole gas temperature is higher than the lattice temperature. In the case $i = 400$ nA, the sample cannot be cooled below 0.8 K at all. The standard measurement current of 100 nA will cause a deviation of the hole temperature from the lattice temperature when the temperature is below 0.7 K, but does not saturate as the lattice temperature is reduced to 0.35 K, the minimum possible value. At 20 nA, hole gas and lattice temperature agree at all possible temperature values.

2.3.3 External heat sources

External heat sources can either heat the electron gas directly or by heating its surroundings. Direct heating is similar to the current heating mentioned above, because electron-lattice energy relaxation forms the bottleneck for cooling. Since it is not dependent on the measuring current, the gas temperature is independent of the excitation current if $P_{\text{ext}} \gg P_{\text{current}}$. An example for an external heat source is a gate leakage current which injects hot carriers into the channel and causes ohmic heating when it flows back to the gate voltage source.

If the external heat source is powerful enough, it can also heat the sample stage (or parts of it). This becomes a severe problem when the thermometer is located far away from the sample. The result is that the thermometer will correctly report its own temperature. However, this temperature does not reflect the sample temperature.
Chapter 3

Band Structure and Effective Mass

The effective mass of holes in Ge is a very interesting parameter. Already in bulk Ge, the hole bands are non-parabolic and anisotropic. The effective mass therefore depends both on direction and energy. When a thin film of Ge is formed inside a SiGe compound, two additional effects modify the dispersion relation. The confinement removes translational invariance in the z-direction. Due to their higher out-of-plane mass, heavy holes (HH) have a lower confinement energy than light holes (LH), so that it is possible to populate the well only with heavy holes. Applying compressive strain to the Ge layer has the same effect.

As a result of lifting the LH-HH degeneracy, strain and confinement both decrease the in-plane mass of the heavy holes. One has to keep in mind that the different masses of heavy and light holes are due to the interaction between the bands in the first place. The lifting of the degeneracy reduces this interaction.

As a structural parameter, the effective mass can be expected to be independent of the sample mobility. The latter is mainly determined by impurities of the sample, while the former depends on the main constituents of the sample only. It is therefore possible to compare effective masses of samples with widely different mobility.

In this chapter, the hole picture is used throughout, i.e., the energy scale is the energy of the holes. In figures, the valence band will therefore be above the band gap, and holes will preferably occupy states with the lowest energy.
Fig. 3.1: Valence band offset for pseudomorphically strained Si$_{1-x}$Ge$_x$ on a relaxed Si$_{1-y}$Ge$_y$ substrate. Holes can be confined to the strained layer if its Ge content is higher than that of the substrate. The quantum well depth can be approximated by $\Delta E_V \approx 750$ meV$(x - y)$. Taken from Rieger and Vogl [38]

3.1 The Parabolic Case

Assuming that the 3-dimensional band can be described by the same constant effective mass $m^*$ in both channel and cladding, the Schrödinger equation of a quantum well created by the potential $V(z)$,

$$\frac{p^2}{2m^*} \Psi + V(z) \Psi = E \Psi,$$  \hspace{1cm} (3.1)
can be solved by a product ansatz \( \Psi = \exp[ikr] \psi(z) \). Here and in the following, bold face symbols denote 2-dimensional vectors in the \( x-y \) plane. The energy eigenvalues \( E \) are given by

\[
E = \frac{\hbar^2 k^2}{2m^*} + \epsilon_z
\]  

(3.2)

where \( \epsilon_z \) is an eigenvalue of the one-dimensional Schrödinger equation

\[
\epsilon_z \psi(z) = \left( \frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V(z) \right) \psi(z).
\]  

(3.3)

For bound states the eigenvalues are discrete and are enumerated by \( n = 0, 1, \ldots N_z \), ascending in energy. For finite quantum well depth, the number \( N_z \) of these eigenvalues is finite, but there is always at least one such state. Each of the eigenvalues is associated with a subband with dispersion \( \epsilon_k = k^2/2m^* \) in the \( x-y \) plane. The \( B = 0 \) density of states

\[
g(\epsilon) = \frac{m^*}{\pi \hbar^2} \sum_{n=0}^{N_z} \Theta(\epsilon - \epsilon_n)
\]  

(3.4)

is a staircase function, where \( \Theta \) is the unit step function.

Including a magnetic field in \( z \)-direction, with vector potential \( A \), the momentum operator \( p \) is replaced by

\[
p \rightarrow p - eA.
\]  

(3.5)

Choosing of the vector potential as

\[
A = (0, xB_z, 0) \\
B = \text{rot}A = (0, 0, B_z)
\]  

(3.6)

the Hamiltonian becomes

\[
H = \frac{1}{2m^*} \left[ -\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + (\hbar k_y - exB_z)^2 \right] + \frac{\hbar^2 k_z^2}{2m^*} + V(z).
\]  

(3.7)

The term in square brackets is a harmonic oscillator in \( x \)-direction, and the rest of the equation a one-dimensional quantum well, so that the Schrödinger equation has eigenvalues

\[
\epsilon(N) = \frac{\hbar eB}{m^*} (N + \frac{1}{2}) + \epsilon_z
\]  

(3.8)

where \( \epsilon_z \) is the \( B \)-independent localization energy calculated in (3.3) and \( N \) is the Landau level number. The degeneracy of a Landau level (including spin) equals \( N_L = 2eB/\hbar \), so
that the number $\nu$ of occupied Landau levels is $\nu = p_s h/2eB$. Thus, at a finite $B$-field the density of states has the form

$$g(\varepsilon) = N_L \sum_{N=0}^{\infty} \delta(\varepsilon - \varepsilon_0 - \hbar \omega_c (N + \frac{1}{2}))$$

In an experiment, measurement of the Landau level separation is used to determine the effective mass (see section 3.6). In non-parabolic bands the picture becomes more complicated, as will be discussed in the following.

### 3.2 Calculation: Envelope function approximation

The calculation of the energy levels of semiconductor heterostructures is based on the perturbative treatment introduced by Luttinger [39, 40]. Although originally devised to treat only slowly varying background potentials $V$ or the influence of magnetic fields, the scheme has proven to be applicable to rapidly changing potentials as well [41]. Even changes to the band structure parameters of the theory ($\gamma_{1,2,3}$) can be treated. Care has to be taken when doing so to preserve the hermitian property of the Hamiltonian.

Luttingers approach was to absorb rapid variations of the wave function, leaving only the long range modulation in what can be looked at as an extended version of the $\vec{k} \cdot \vec{p}$ method. This property has given the method the name “Envelope Function Approximation” (EFA). Various subtypes are possible depending on the choice of bands used. For electrical transport in the hole bands of group IV and III-V semiconductors taking into account the 6 hole bands (including spin) is sufficient.

The $6 \times 6$ Envelope Function Approximation (EFA-) Hamiltonian $H_k$ is defined by [42]

$$H_k = \begin{pmatrix}
P + Q & S & R & 0 & -S\sqrt{2} & -R\sqrt{2} \\
S^\dagger & P - Q & 0 & R & Q\sqrt{2} & S\sqrt{3/2} \\
R^\dagger & 0 & P - Q & -S & S^\dagger\sqrt{3/2} & -Q\sqrt{2} \\
0 & R^\dagger & -S^\dagger & P + Q & R^\dagger\sqrt{2} & -S^\dagger/\sqrt{2} \\
-S^\dagger/\sqrt{2} & Q\sqrt{2} & S\sqrt{3/2} & R\sqrt{2} & P + \Delta_0 & 0 \\
-R^\dagger\sqrt{2} & S^\dagger\sqrt{3/2} & -Q\sqrt{2} & -S/\sqrt{2} & 0 & P + \Delta_0
\end{pmatrix}$$

(3.10)

It takes into account heavy holes (HH), light holes (LH) and spin split off (SO) holes.
3.2. CALCULATION: ENVELOPE FUNCTION APPROXIMATION

the bulk, the parameters are given by

\[ P = \frac{\hbar^2}{2m_0} \gamma_1 (k_x^2 + k_y^2 + k_z^2) + P_\epsilon + V \]
\[ Q = \frac{\hbar^2}{2m_0} \gamma_2 (k_x^2 + k_y^2 - 2k_z^2) + Q_\epsilon \]
\[ R = -\frac{\hbar^2}{2m_0} \frac{\sqrt{3}}{2} \left[ (\gamma_1 + \gamma_3) k_z^2 + (\gamma_2 - \gamma_3) k_+^2 \right] \]
\[ S = -\frac{\hbar^2}{2m_0} 2\sqrt{3} \gamma_3 k_- k_z \]
\[ k_+ = k_x + ik_y \]
\[ k_- = k_x - ik_y \]

The strain dependent matrix elements \( P_\epsilon, Q_\epsilon \) are defined as

\[ P_\epsilon = -D_d (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \]
\[ Q_\epsilon = -\frac{1}{3} D_u (\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz}) \]

where \( D_d \) is the hydrostatic strain matrix element and \( D_u \) is the uniaxial strain matrix element. In the hole picture, uniaxial compressive strain with \( \epsilon_{xx} = \epsilon_{yy} < 0 \) and \( \epsilon_{zz} > 0 \) increases the energy of the light hole states compared to the heavy hole states (in the hole energy scale). In Ge/Si\(_{0.3}\)Ge\(_{0.7}\) – heterostructures, this mechanism is the major contributor to HH-LH splitting which amounts to 100 meV. In AlGaAs/GaAs heterostructures, strain is negligible and the splitting is mostly due to the different localization energy of heavy and light holes. Strain splitting of the LH and HH states is due to the term \( Q_\epsilon \) which also changes the mixing between LH and SO states. The term \( P_\epsilon \) only changes the effective well depth and acts only as an additional confinement potential.

It should be kept in mind that the matrix is an operator, acting on the six-dimensional wave function \( \Psi(k) \). In the bulk, where the matrix elements are position independent, the dispersion relation can easily be found by diagonalizing the matrix \( H_k \), since in this case \( k \) is just a parameter.

In the case of a heterostructure grown along the \( z \)-axis, however, where \( \gamma_i = \gamma_i(z) \), we have to go back to the operator description by letting \( k_z \to i\partial/\partial z \). Furthermore, to keep the Hamiltonian hermitian, we have to replace

\[ \gamma k_z^2 \to -\frac{\partial}{\partial z} \gamma(z) \frac{\partial}{\partial z} \]
\[ \gamma k_z \to \frac{i}{2} \left( \frac{\partial}{\partial z} \gamma(z) + \gamma(z) \frac{\partial}{\partial z} \right) \]
We further describe the band offsets and the electrical potentials by having a position dependent term \( V \).

Please note that band warping is brought about solely by the term

\[
(\gamma_2 - \gamma_3)k_z^2
\]

in \( R \) ("warping term"). If the warping term is left away from \( (3.11) \), the matrix is invariant under rotations around the \( z \)-axis. Therefore, in this approximation constant energy surfaces are circles. This fact plays a major role when calculating Landau levels using the \( 6 \times 6 \) EFA Hamiltonian. Landau levels are usually calculated in the "axial approximation", meaning that the warping term has been neglected.

### 3.3 Numerical solution

For numerical calculations, a basis set has to be introduced. We choose a basis \( \psi_m(k) = u_m \exp(ik z) \), where \( m = 1 \ldots 6 \) enumerates the components corresponding to the spin wave function and \( u_m \in \mathbb{C} \). The \( k_z \) are chosen according to \( k_z = j/(2\pi L), j = 0 \ldots N - 1 \) where \( L \) is the length of the calculation interval. We choose the calculation interval to be the channel \( \pm 10 \) nm of cladding. Note that this particular choice of the basis actually implies periodic boundary conditions, shown in Fig. 3.3. This means that implicitly we calculate the miniband structure of a superlattice of periodicity \( L \). For the ground state and the lowest excited states, this is no problem, since the overlap between the wave functions in adjacent wells is sufficiently small. For other states, particularly those that are not confined to the well, the wave function is distorted. The number \( 6N \) of basis functions determines the effort needed for a solution, which is proportional to \( N^3 \) (diagonalization of a full matrix).

We can now construct the matrix \( H_{m,m'}(k_z,k'_z) \). For example, the matrix element

\[
H_{1,3}(k_z,k'_z) = \langle \frac{3}{2} \frac{3}{2}, k'_z | H | k_z, \frac{3}{2} \frac{1}{2} \rangle
\]

would be

\[
R^1(k_z,k'_z) = -\frac{3\hbar^2}{4m_0} \left[ (\gamma_2(k_z - k'_z) + \gamma_3(k_z - k'_z))k_z^2 + (\gamma_2(k_z - k'_z) - \gamma_3(k_z - k'_z))k_z^2 \right]
\]

In this way, we can assemble the whole matrix, but we need the Fourier components of the coefficients, i.e., \( \gamma_i(k_z - k'_z) \). To calculate these Fourier components, we start in the position
3.3. NUMERICAL SOLUTION

Fig. 3.2: The first (red) and second (blue) heavy hole subbands are confined to the quantum wells, while the first light hole subband (green) is confined only in the left example, which is due to the lower confinement energy (wider channel). In both examples, only the lowest subband is located below the Fermi energy (dashed lines). The shape of the light hole wave function outside the right well is not realistic, since for unbound states the periodic boundary conditions lead to artifacts (see also Fig. 3.3). Due to strain, the potential well is shallower for light holes (dashed line) than for heavy holes (thick solid line). The kink of the potential at $z = 6$ nm in the right panel signifies the location of the doping spike, set to have the same carrier density as the hole gas in the well. In the left example, the spike is located at $z = 0$. $n_1$ denotes the areal density of ionized dopants in the doping spike.

representation, using equidistant points to sample the position dependent parameters. We then obtain their Fourier components by a discrete Fourier transform. Then, the matrix $H_{i,i'}(k_z,k'_z)$ is assembled and transformed back into position space by the inverse discrete Fourier transform. Then, we calculate the eigenvalues.

The in-plane band structure is found by assembling the matrix for any $(k_x, k_y)$ a solution is to be sought for and solved. A $N = 128$ solution (finding eigenvalues and eigenvectors of a $768 \times 768$ matrix) takes about 5 minutes on a standard PC.
Fig. 3.3: The periodic nature of the basis set chosen for the calculation means that the calculation effectively yields the energy levels of a superlattice like the one shown. Bound states with energy lower than the cladding potential are hardly affected (red, blue). States with energy above the minimum of the cladding potential (green) are not confined to the well and are not calculated correctly.

3.4 Self consistency

The solution to the Schrödinger equation with a given potential results in a charge distribution which in turn produces an electrostatic potential. For a physical solution of the problem, it must be assured that the two potentials are identical. To facilitate solution, the problem is split up. The Schrödinger problem is solved assuming a given charge density in the channel and assuming an electric field 10 nm from the left channel-cladding interface, which happens to be the left border of the calculation interval ($x = 0$ in the left hand example of Fig. 3.2). The calculation assumes that the only charges are the doping spike and the charge distribution of the hole gas in channel. Homogeneously distributed charges are not taken into account.

Only the state with $k_\parallel = 0$ is used for the self consistent calculation. This treatment is justified because the charge distribution of states with $k_\parallel \neq 0$ is sufficiently similar to the charge distribution for $k_\parallel = 0$. Furthermore, the aim of the calculation is to make predictions about the effective mass. As is known both from experiments and calculations, the effective mass is very similar for single sided (asymmetric) and double sided (symmetric) doping. This clearly shows that smaller changes in the potential cannot significantly influence the effective mass. The level of self consistency used here is therefore entirely sufficient for the purpose of determining the effective mass by calculations.

Starting with a reasonably realistic potential $V_1$, the program determines the charge distri-
3.5 LANDAU LEVEL CALCULATION

bution by solving the Schrödinger equation. From this charge distribution the electrostatic potential $V'$ can be calculated. To ensure convergence, the potential for the next iteration is calculated according to $V_{n+1} = \alpha V' + (1 - \alpha)V_n$, where $0 < \alpha \leq 1$ is an adjustable parameter. The decay constant $\alpha$ is chosen manually to obtain rapid convergence while avoiding oscillatory behavior of sequential iterations.

The second part of the solution is to find suitable values for the electric field at the border of the calculation interval. The right border is assumed to face the bulk SiGe material. The electrostatic field at this point is given by the depletion charge underneath the channel. Except for the first 50-100 nm underneath the channel, which are grown using different plasma conditions, it is reasonable to assume a constant impurity concentration. For details of the growth method, see appendix [3]. No measurements of the impurity concentration of the material underneath the channel exist, so that one is forced to estimate the concentration. Assuming reasonable values of the impurity concentration, this charge is on the order of $10^{11} \text{ cm}^{-2}$.

The depletion charge underneath the channel is considered constant throughout the iteration process that establishes self-consistency. The reason is the following: the depletion charge is dependent on the difference between the bulk valence band energy and the valence band energy directly below the lower interface, which is on the order of 250 meV for a p-type background and 600 meV for a n-type background, and changes only by 5-10 meV during the iteration process. This variation is smaller than the error in the estimated impurity concentration. Therefore, this treatment is justified. Since the charge density underneath the channel is small compared to the charge in channel and doping, the shape of the potential well is not affected much by the choice of the impurity concentration, and the effect on the effective mass is negligible.

3.5 Landau level calculation

The replacement of the momentum operator (3.5) in the Hamiltonian (3.10) can be shown to be equivalent to replacing the operator $k_-$ by the Landau level lowering operator $a_-$, and $k_+$ by the Landau level increasing operator $a_+$ according to [43]

$$k_\pm \rightarrow \frac{\sqrt{2}}{\lambda_c} a_\pm$$  \hspace{1cm} (3.19)

where the magnetic length $\lambda_c = \sqrt{eB/\hbar}$ is the characteristic size of the state in the field, i.e., the quantum mechanical equivalent of the cyclotron radius in classical mechanics. With the exception of the warping term (3.16), the Landau level lowering operator always
appears in a position in (3.10) that associates it with a spin raising operation. The equivalent is valid for the Landau level raising operator $a_+$. In other words, the sum of Landau level number and spin projection onto the $z$-axis is conserved. This is a result of the underlying Hamiltonian being invariant under rotations around the $z$-axis.\(^1\)

Neglecting the warping term reduces the computational complexity of the system, since only at most six states can be connected. The actual number is reduced when some states with $N = 0$ are involved, because further lowering of the Landau level is impossible. If the warping term is kept, an infinite number of states is connected. We have investigated how the omission of the warping term influences the structure of the Landau levels and the effective mass by first calculating the Landau levels in the axial approximation and then including the warping term as a perturbation. We find that there is no noticeable impact of inclusion of this term. Interestingly, this is very different from the pronounced effect the warping term does have on the shape of the zero-field bands, particularly at high carrier density.

### 3.6 Measuring the effective mass

The effective mass inside a 2-dimensional hole gas can be measured either by cyclotron resonance or by the temperature dependence of the Shubnikov–de Haas (SdH) oscillations. Both methods use a magnetic field to effect the formation of Landau levels. Cyclotron resonance directly measures the transition energy between Landau levels and has the potential to measure the mass as function of $B$. From Shubnikov–de Haas oscillations the mass is deduced from the temperature dependence of the amplitude of the oscillations, a method that introduces some averaging but typically works at lower fields and is a pure electrical transport measurement. The relative ease of SdH experiments is the reason most masses are measured this way. The following will concentrate only on this technique.

In zero magnetic field the effective mass is directly related to the two-dimensional density of states (DOS), $g(\varepsilon_F)$, by

$$m_{\text{DOS}}^* = \pi \hbar^2 g(\varepsilon_F) = \frac{\hbar^2}{2\pi} \int_{\varepsilon = \varepsilon_F} \frac{1}{|\nabla_k\varepsilon|} \, dk,$$

where the integral is taken along a Fermi energy contour. In the simplest case of parabolic bands the DOS mass defined by (3.20) is just a constant, whereas in the more general case of non-parabolic bands $m^*$ depends on energy and hence on carrier density. Since it is a measure of the DOS at the Fermi level, $m^*$ is directly related to very important quantities,\(^1\) which is hard to see even at a third glance.
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particularly the carrier mobility $\mu$. The latter is influenced both directly through $\mu = e\tau/m^*$, where $\tau$ is the carrier scattering time, and indirectly through the screening of scattering centers (see also chapter 4.2).

Experimentally, it is very hard to directly access $m^*_{\text{DOS}}$. As mentioned above, $m^*$ is usually derived from a cyclotron resonance (CR) experiment, or, more easily, from the temperature dependence of the oscillatory part of the magneto-resistance, the so-called Shubnikov-de Haas oscillations. Both measurements yield the cyclotron frequency $\omega_c$. In the limit of $B \to 0$, $\omega_c$ is given by

$$T_c = 2\pi/\omega_c = \frac{\hbar^2}{eB_z} \int_{\epsilon=\epsilon_F} \frac{1}{|\nabla_{\epsilon}\xi|} d\epsilon.$$  \hspace{1cm} (3.21)

and in this limit the definition $\hbar\omega_c = \hbar eB_z/m^*$ of the effective mass $m^*$ is identical to (3.20). For parabolic bands, where $m^*$ is independent of energy, the equality of the two definitions of the effective mass holds for arbitrarily high magnetic fields, even though (3.21) is not valid for strong magnetic fields.

For hole bands in most semiconductors a strong nonparabolicity exists. This means that the 2-dimensional density of states is not independent of energy. In SiGe, the DOS mass $m^*_{\text{DOS}}$ increases with hole kinetic energy. The Hamiltonian can thus no longer be brought to the form of a harmonic oscillator as in (3.7). Consequently, the Landau levels are no longer distributed equally along the energy axis and naturally the question arises to what extent the Landau level spacing still reflects the DOS mass (3.20). The experimental problem one has to face is that both SdH and CR experiments require $\omega_c\tau \gtrsim 1$, where in general (3.21) does not hold. In SiGe, a magnetic field of about 1 T is required even for the best samples. Before the returning to the issue of different definitions of the effective mass, we will first show how the effective mass is determined from SdH oscillations, and how our calculations of the Landau level energy can be used to link DOS mass and SdH mass.

Landau levels have a finite width due to lifetime (homogeneous) broadening which is due to scattering from impurities and phonons and gives a Lorentzian peak shape. When averaging over a macroscopic sample, inhomogeneous broadening of the Landau levels can also play a role. It is brought about by a spatial average over the localization energy $\epsilon_0$. When inhomogeneous broadening dominates, the peak shape depends on the particular distribution of $\epsilon_0$. Thus, in a magnetic field the DOS is a superposition of broadened peaks centered around Landau level positions, as depicted in Fig. 3.4. In the following we will use only homogeneous broadening, as experimental observations show that it is the dominant contribution.

Smrčka and Středa [44] showed that the conductivity $\sigma_{ij}$ at finite temperature can be
Fig. 3.4: The lifetime broadened Landau levels are centered around the position derived from $6 \times 6$ EFA calculations (left panel). The superposition of the individual peaks yields the DOS (right panel). To determine the resistance oscillations (Shubnikov–de Haas oscillations), the convolution with the derivative of the Fermi function (shown for $T = 2$ K) is calculated. The sudden increase of the DOS in the right panel above -0.07 eV is due to the second HH subband (not shown in the left panel to improve legibility).

expressed as

$$\sigma_{ij}(\mu, T) = \int_{-\infty}^{\infty} \frac{df}{d\epsilon}(\epsilon, \mu, T)\sigma_{ij}(\epsilon, T = 0)$$

(3.22)

$$\sigma_{xx}(\epsilon, 0) = \frac{e^2}{m^*} \frac{\tau}{1 + \omega^2 \tau^2} N_{\parallel}$$

(3.23)

$$\sigma_{xy}(\epsilon, 0) = e\frac{\partial N}{\partial B}\bigg|_{\epsilon} - \omega_c \tau \sigma_{xx}(\epsilon, 0)$$

(3.24)

where $N_{\parallel}$ is the number of states participating in 2-dimensional transport and $N$ is the number of states below the electrochemical potential $\mu$. The scattering time $\tau$ is the quantum mechanical lifetime of a state, which was assumed to be the same as the transport scattering time in the derivation. Since the two are generally different from each other, the formula has to be adapted. In fact, the explicit occurrences of $\tau$ in (3.23) and (3.24) have to be replaced by the transport scattering time $\tau_{tr}$. The quantum lifetime, which is responsible for the broadening of the Landau levels, is hidden in $N$ and $N_{\parallel}$. Using the density of states $g(\epsilon) = g_0 + \Delta g(\epsilon)$, where $g_0$ is the zero-field value and $\Delta g(\epsilon)$ is the deviation from the zero-field value associated with the formation of Landau levels (see also
Fig. 3.4, gives \[45\]

\[ N_{\parallel}(\epsilon) = p_s \left( 1 + \frac{\Delta g(\epsilon)}{g_0} \right) \]  

(3.25)

The field dependent resistivity \( \rho(B) \) is then calculated by inversion of the conductivity tensor \( \sigma_{ij}(\mu, T) \) in (3.22) to yield

\[
\rho_{xx} = \rho_0 \left( 1 + 2 \frac{\Delta g}{g_0} \right) \\
\rho_{xy} = \rho_0 \omega_c \tau_0 \left( 1 - \frac{1}{\omega_c^2 \tau_0^2} \frac{\Delta g}{g_0} \right),
\]

(3.26)

(3.27)

As is easily seen, the field dependence of the resistance results from the variable density of states at the Fermi level. Assuming homogeneous broadening of the Landau levels, the modulation of the electrical resistance is calculated as \([44, 45]\)

\[
\frac{\Delta \rho}{\rho_0} = 4 \sum_{s=1}^{\infty} \exp \left[-\frac{\pi s}{\omega_c \tau_q}\right] \frac{s \xi}{\sinh(s \xi)} \cos \left(\frac{2 \pi s \epsilon_F}{\hbar \omega_c} - s \pi\right)
\]

(3.28)

where \( \xi = 2\pi^2 k_B T / \hbar \omega_c \). This is, in fact, a Fourier series expansion of a homogeneously broadened density of states convolved with the first derivative of the Fermi distribution function. The first factor in the sum describes homogeneous broadening due to a finite state lifetime \( \tau_q \). Note that this time is different \([46]\) from the Drude transport time \( \tau_{tr} \) defined by \( \sigma = p_s e^2 \tau_{tr} / m^* \). The second term describes a dampening of the modulation due to the finite width of the Fermi function. This dampening enables us to measure the cyclotron energy \( \hbar \omega_c \) in units of \( k_B T \).

Although the derivation of (3.28) assumed a constant effective mass, the equation in fact only relates the resistance to the Landau level spacing \( \hbar \omega_c \) of the few Landau levels that take part in transport at any given \( B \). The periodicity due to the last term of (3.28) does not depend on \( \hbar \omega_c \), even though it appears so in the formula, but reflects the degeneracy of the Landau levels. Thus, even in non-parabolic bands, (3.28) can be used to extract the Landau level spacing, as detailed in the following.

We extract the effective mass from measured Shubnikov–de Haas oscillations by making use of the fact that only the second term in (3.28) is temperature dependent. The effective mass is then calculated using \( \omega_c = eB / m^* \). The justification of the usual association with the zero-field DOS mass will be investigated in the last part of this chapter.

As a simplification, only the \( s = 1 \) term of the sum in (3.28) is kept, which is justified only for small magnetic fields. Thus, if the amplitude of the resistance modulation \( \Delta \rho / \rho_0 \) is measured at several different \( T \) (and all other parameters are kept constant), it is possible
to find the effective mass $m^*$. The procedure of extracting the amplitude is shown in Fig. 3.5: the maxima and minima of the Shubnikov–de Haas oscillations are interpolated, shown in the left panel. At a given field, $\Delta \rho$ is taken as half the distance between the two envelopes. A fit of $\Delta \rho/\rho_0$ at fixed $B$ to the function $C_1 T/ \sinh(C_2 T)$ with $C_1$ and $C_2$ as parameters yields the effective mass, shown in the right panel for three different magnetic fields.

Having found the effective mass $m^*$, it is then possible to determine the lifetime $\tau_q$ of the quantum mechanical states by fitting $x = 1/B$ versus $y = \log(\Delta \rho \sinh(\xi)/\rho_0 \xi)$. This so-called Dingle plot serves not only to determine $\tau_q$, but also to judge the validity of (3.28), because if the assumptions are fulfilled, the experimental data points should form a straight line with an (extrapolated) $y$-axis intercept at $\log(4)$. An example is shown in Fig. 3.6. In the left panel, the Dingle plot of sample 7404-27 is shown to be almost linear, evidencing the homogeneous broadening. The intercept on the $y$-axis is at 1.2, significantly below the theoretical expectation, which is 4. The right panel shows a representative range of Dingle ratios obtained from our samples. It is clearly visible that the Dingle ratios significantly exceed unity, evidencing the predominance of small angle scattering (see also chapter 4).

Figure 3.7 shows experimental masses of Si$_{0.3}$Ge$_{0.7}$/Ge quantum wells. The samples differ widely in channel and spacer width, doping profile and growth method (LEPECVD and MBE). Nevertheless, it is obvious that the experimental mass is an almost linear function
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Fig. 3.6: The Dingle plot of sample 7404-27 (left panel) shows the exponential dependence of the oscillation amplitude on $B^{-1}$ that is associated with homogeneous broadening of the Landau levels. The $y$-axis intercept of 1.2 falls short of the value of 4 predicted by theory. Among others, spin splitting of the Landau levels and parallel conduction [47] (unlikely in this case) can be a cause. High Dingle ratios as shown in the right panel are indicative of predominance of small angle scattering, suggesting a charged impurity scattering mechanism.

of sheet carrier density. Since the effective mass is apparently independent of all sample parameters except material composition and sheet carrier density, it is a very useful quantity to test band structure calculations.

We have calculated the effective DOS mass according to (3.20) from our calculations of the zero-field band structure. It is shown as dashed lines in Fig 3.7. Note that due to Rashba splitting, the lowest HH band is split into two hole bands having different dispersion relations. This splitting depends on the average electric field the wave function experiences. Here, the assumption was that the electric field is essentially zero in the area underneath the channel, as mentioned in section 3.4. According to Gauss’ law the electric field $\mathcal{E}$ rises from near zero at the lower channel interface to about $\mathcal{E} = e\rho_s/\varepsilon\varepsilon_0$ at the upper interface, so that the average electric field experienced by the hole gas is roughly proportional to the carrier density.

According to Fig. 3.7 for sheet carrier densities below $1.0\times10^{12}$ cm$^{-2}$, the DOS mass derived from band structure calculations coincides with the experimental results from SdH measurements. As the carrier density increases further, the calculated DOS mass
Fig. 3.7: The experimental effective mass in Ge/Si$_{0.3}$Ge$_{0.7}$ heterostructures is strongly dependent on sheet carrier density $p_s$. Calculated SdH masses ( layoutParams ) match the experiment, while calculated DOS masses (dashed lines by author, open squares taken from [42]) are significantly larger than experimental data. Due to the asymmetry of the potential well, the lifting of the spin degeneracy leads to two distinct masses for the split bands. Experimental data by the author (▲) and from [48] (● SdH filled circles, ▼ CR).

becomes, however, significantly larger than the experimental cyclotron mass.

The variation of the calculation parameters showed that there is no way to reconcile the calculated DOS mass with the experimental mass. We therefore decided to simulate the whole SdH experiment. The direct calculation of the Landau level energy as function of the magnetic field allows to generate an artificial SdH measurement. To this end, a density of states at zero temperature is derived by homogeneously broadening every Landau level (Fig. 3.4 right panel), using one quantum scattering time $\tau_q$ for all Landau levels and magnetic fields. Then the Fermi energy is determined such that the carrier density remains constant at the selected value.
Fig. 3.8: The comparison of the calculated effective DOS in panel (a) with measured SdH oscillations in panel (b) shows excellent agreement at a carrier density $p_s = 4.58 \times 10^{11} \text{ cm}^{-2}$ and a quantum scattering time $\tau_q = 0.6 \text{ ps}$. Several temperatures are shown, with the oscillations decreasing as the temperature rises from 2.0 K to 5.0 K in steps of 1.0 K. A slowly varying background has been subtracted. Vertical lines in panel (a) indicate the center positions of the calculated Landau levels.

For the determination of $\omega_c$ according to (3.28), and from it the effective mass, only the ratio of $\Delta g/g_0$ is required. The smearing by the thermal distribution is taken into account
in analogy to (3.22) by calculating the effective DOS \( g(\mu, T) \) according to

\[
g(\mu, T) = \int g(0, \varepsilon) \frac{\partial f}{\partial \varepsilon}(T, \varepsilon, \mu)
\]

(3.29)

From the effective DOS, the amplitude \( \Delta g \) is extracted in the same way as from measurements. The only adaptation required is the missing prefactor 2 that causes the resistance oscillations to be twice as large as the DOS oscillations that cause it, according to (3.26).

The result of the calculation is shown in Fig. 3.8 from which we can calculate the amplitude of the SdH oscillations. These oscillations can then be evaluated using the same methods as for experimental results, which provides a high degree of realism. Indeed, as one determines the effective mass in this way, the results closely match those found from the experiment. If anything, the theoretical SdH mass tends to be a little lower than the experimental mass. In contrast to the SdH mass, the zero-field DOS mass agrees with the experiment only for carrier densities below \( 1.0 \times 10^{12} \text{ cm}^{-2} \). For higher densities, the zero-field DOS mass becomes significantly larger than the measured SdH mass. We therefore arrive at the important result that high carrier density devices have higher effective masses and lower mobility when operated at zero magnetic field than one would predict from SdH measurements. Particularly, the phonon-limited mobility, behaving as \((m^*)^{-2}\) [49, 50], is expected to be reduced.

Due to the asymmetry of the potential well, the spin degeneracy of the zero-field band is lifted and the two bands have different effective masses (dashed curves in Fig. 3.7). No such feature is observed from the SdH mass, probably because the effect is suppressed by the Zeeman effect. Only for extremely high carrier densities, beating of the SdH oscillations could be observed, which is the hallmark of band splitting. In contrast to experiment, calculations enable us to separate the oscillations of the two sets of Landau levels that are split by the Rashba effect. We can then separately determine the effective masses. We find that they differ only slightly from each other except at very high carrier density. As an example, for \( p_s = 2.1 \times 10^{12} \text{ cm}^{-2} \) the mass found is 0.184 \( m_e \) from SdH oscillations and 0.268 \( m_e \) from the DOS for one band and 0.169 \( m_e \) from SdH oscillations and 0.227 \( m_e \) from DOS for the other band. The relative mass difference \( \Delta m/\bar{m} \) is 16.5\% for the DOS mass, while it is only 8.5\% for the SdH mass.

The calculated effective mass is also a function of the quantum well width. As the channel width is decreased, the effective mass increases. This effect is explained by an increasing probability of the carriers to be in the barrier, where the effective mass is higher. The structures studied here have well widths above 8 nm, where the mass change is within the experimental spread. However, if the well width were reduced significantly, i.e. to 5 nm and less, the effective mass is expected to increase dramatically. The mobility of
Si$_{0.2}$Ge$_{0.8}$/Si$_{0.5}$Ge$_{0.5}$–samples with various channel widths has been investigated by Tsujiino et al. [15], but no effective masses were published. Since the mobility was below 2000 cm$^2$/Vs for channel widths below 5 nm, SdH measurements were probably not done. Mobility data on such narrow wells with pure Ge channels have been published by Irisawa et al. [51], but again, no effective mass was published.
Chapter 4

Mobility

The mobility of the confined carriers in the plane is one of the most important properties of a sample and is usually the parameter that is used to distinguish “good” from “bad” samples. At room temperature and above, the mobility of carriers in silicon and germanium is largely determined by phonon scattering. As the temperature is decreased, phonon scattering is reduced and the mobility is governed by structural properties of the sample, in particular intentional and unintentional doping as well as point defects of the lattice. Two-dimensional confinement of the carriers leads to a further type of scattering related to interface quality of the channel. This includes interface roughness and charged impurities or defects that are localized at the interface.

The mobility of hole gases in strained germanium channels depends on the carrier density. The highest values reported in literature are 120'000 cm$^2$/Vs at 8.5×10$^{11}$ cm$^{-2}$ [52] and 89'000 cm$^2$/Vs at 6.0×10$^{11}$ cm$^{-2}$ [12], both grown by LEPECVD. The highest mobility of MBE grown samples was 55'000 cm$^2$/Vs at 5.1×10$^{11}$ cm$^{-2}$ [53]. At higher carrier densities, the mobility has remained somewhat lower, 26’000 cm$^2$/Vs at 1.05×10$^{12}$ cm$^{-2}$, 34’000 cm$^2$/Vs at 1.6×10$^{12}$ cm$^{-2}$ and 26’600 cm$^2$/Vs at 1.9×10$^{12}$ cm$^{-2}$ [54].

The mobility $\mu$ is defined as $\mu = e\tau_{tr}/m^*$, where $\tau_{tr}$ is the momentum relaxation time and $m^*$ is the effective mass of the carriers. Since the longitudinal conductivity $\sigma_{xx}$ depends on the mobility $\mu$ and the carrier density $p_s$ according to $\sigma = e\mu p_s$, the mobility is determined from a resistivity measurement using the equivalent formula $\mu = R_H/\rho_0$, where $\rho_0$ is the zero-$B$ resistivity and the Hall constant $R_H = (ep_s)^{-1}$ is determined from the transverse resistance $\rho_{xy}(B) = R_H B$.

When treating the effects of doping, the question whether the supply layer (doping) of a quantum well should be above or underneath the channel may seem arbitrary at first. However, the properties of upper and lower interfaces are different, particularly when the
Fig. 4.1: Among others, the geometrical structure of the sample can have a great influence on the mobility, because it determines where the wave function will be located. The surface pinning of the Fermi level is indicated by the blue square to the left. Doping underneath the channel (“inverted doping”, left side) pulls the wave function toward the lower interface, while doping between channel and surface (“normal doping”, right side) pulls the wavefunction up.

channel is under compressive strain, as is the case for lattice-matched germanium on a relaxed silicon-germanium alloy. In addition, one has to make sure that intentional doping of the supply layer is not followed by unintentional doping of the channel when doping is done underneath, for example by segregation.

In the following we will first lay out the theoretical background of scattering and screening in two dimensions. The results are then applied to the experimental mobility of LEPECVD grown quantum wells, showing the main scattering parameters and highlighting the importance of interface impurity scattering to SiGe/Ge heterostructures in general.

In the theoretical treatment of the mobility, the simplification of assuming a circular Fermi surface is used throughout. Modifications due to the warping of the band structure are a relatively small effect, smaller than the experimental spread of measured mobilities. Therefore it seems justified not to take band warping into account in this chapter. The impact of band warping on the magnetoresistance will be treated in chapter 5.

4.1 Scattering

In semiconductor heterostructures, the natural description of eigenstates of the Hamiltonian are 2-dimensional plane waves in the \((x,y)\)-plane with quantization in the third \((z)\) direction, i.e. \(\Psi(\vec{r}) = A^{1/2} \phi(z) \exp(ikr) = |k\rangle\), using \(A\) as the normalization area. Here, \(\vec{r} = (x,y)\), \(\vec{k} = (k_x, k_y)\) and \(k = k_z\) (the subscript is frequently omitted). Since transla-
tional invariance in the $x$-$y$ plane is destroyed by both structural imperfections and lattice vibrations (phonons), these states have only a finite lifetime. At low temperatures, phonon scattering plays only a minor role. We thus concentrate on the elastic scattering due to impurities and interface roughness. For time-independent scatterers, Fermi’s Golden Rule tells us that the transition rate $w(k)$ out of the state with wave vector $k$ is related to the matrix element $\langle k' | V | k \rangle$ between the incoming wave $| k \rangle$ and the outgoing wave $| k' \rangle$ by

$$
\frac{1}{\tau(k)} = w(k) = \frac{2\pi}{\hbar} \int \frac{d^2k'}{(2\pi)^2} \delta(\epsilon_{k'} - \epsilon_k) |\langle k' | V | k \rangle|^2
$$

(4.1)

$$
= \frac{m^*}{2\pi\hbar^2 k_F} \int A d^2k' \delta(k' - k_F) \times
$$

$$
\times \left| \int A \frac{d^2r}{A} \int_{-\infty}^{\infty} dz e^{iqr} |\phi(z)|^2 V(r, z) \right|^2
$$

(4.2)

Here, we make the further assumption that the scattering is isotropic in the sense that the scattering cross section does not depend on the direction of the scattering wave vector $q = k - k'$, but only on its magnitude. It is then possible to express the scattering by the magnitude of $q$ alone, and we change the parameter for the integration around the Fermi surface to the scattering angle $\theta$:

$$
w(k) = \frac{m^*}{2\pi\hbar^2 k_F} \int_0^\pi d\theta k_F A |V(q)|^2
$$

(4.3)

$$
V(q) = \int A \frac{d^2r}{A} \int_{-\infty}^{\infty} dz e^{iqr} |\phi(z)|^2 V(r, z)
$$

(4.4)

The structure factor

$$
S(q) = A|V(q)|^2
$$

(4.5)

describing the strength of the scattering is calculated as an integral over the whole impurity potential $V$. In our case one is dealing with individual scatterers with identical scattering potentials $V'$ that are randomly distributed in the sample in the form of a 2-dimensional sheet at position $z$ with 2-dimensional density $N$ and without statistical correlation. The total scattering potential $V$ is then given by

$$
V(r, z) = \int d^2 r' \sum_i \delta(r_i - r + r') V'(r', z)
$$

(4.6)

where the $r_i$ denote the positions of the scattering centers. Upon averaging over the impurity distribution, the impurity averaged structure factor is given as

$$
S(q) = N|V'(q)|^2
$$

(4.7)
where $V'(q)$ is the Fourier transform of a single scattering potential $V'(x)$, defined by

$$V'(q) = \int d^2r \int_{-\infty}^{\infty} dze^{iqr}|\phi(z)|^2V'(r,z). \quad (4.8)$$

As pointed out by Monroe et al. [55], absence of long range statistical correlations is important here, ensuring that the structure factor (and, therefore, the scattering rate) is independent of the sample size. This is equivalent to saying that scattering rates from different sources can simply be added.

As mentioned, the distribution was assumed to be 2-dimensional. In view of the foregoing assumption that scattering rates can be added, a 3-dimensional distribution can be taken into account simply by first calculating the rate sheet by sheet and then integrating over the third coordinate. We will make use of this fact when calculating the scattering rate associated to homogeneously distributed coulomb scatterers.

The particle lifetime denotes how rapidly a quasiparticle decays. However, not all scattering events are of equal importance for a certain physical quantity. Current transport through a sample is effected by shifting the whole Fermi surface. Relaxation of a current requires shifting the Fermi surface back to the equilibrium position, i.e. relaxing the net momentum of the Fermi surface. Assuming a well defined Fermi surface, the momentum relaxation is $\Delta p = p_F(1 - \cos \theta)$, where $\theta$ is the scattering angle. Changing the integration variable from $\theta$ to $q = 2k_F\sqrt{1 - \cos \theta}$, the current relaxation time $\tau_{tr}$ is written as

$$\frac{1}{\tau_{tr}} = \frac{m^*}{\pi \hbar^3 k_F} \int_0^{2k_F} \frac{S(q) dq}{\sqrt{1 - q^2/4k_F^2}} q^2 \quad (4.9)$$

while the quasiparticle relaxation time is

$$\frac{1}{\tau_q} = \frac{m^*}{\pi \hbar^3 k_F} \int_0^{2k_F} \frac{S(q) dq}{\sqrt{1 - q^2/4k_F^2}} \quad (4.10)$$

The ratio $\alpha = \tau_{tr}/\tau_q$ is called Dingle ratio. It is unity for isotropic scattering, while dominance of small angle scattering results in a Dingle ratio much larger than one. Since the observation of Shubnikov–de Haas oscillations permits the determination of $\tau_{tr}$ and $\tau_q$, it is used to determine the dominant scattering mechanism(s) in a given sample.

### 4.2 Screening of scattering potentials

The screening of the scattering potential is of importance for the scattering cross section, since screening can not only reduce the scattering cross section, but also change the shape
of the scattering potential. Amongst other effects, this can lead to a different relation of the mobility on adjustable parameters like the sheet carrier density. Here, screening is treated in the linear response regime, where the density response to a disturbance is assumed to be linear in the perturbation.

### 4.2.1 Density response function $\chi$

The density response function $\chi(q)$ describes the density change $\rho(q)$ that is induced by an internal perturbation potential $V(q)$, according to $\rho(q) = \chi(q)V(q)$. It is also called polarisability. The internal potential includes all screening effects. Assuming this potential is given, the resulting density response is calculated in the following. The results of this section are then used in section 4.2.2 to calculate the response to an external potential. In a first approximation, one neglects exchange and correlation effects and treats the gas as non-interacting. The noninteracting density response function is usually denoted by $\chi^0$. For long wave perturbations (small $q$), one finds $\chi^0(q) = g(\epsilon_F)$, where $g$ is the density of states. This is the Thomas-Fermi approach.

To get a more realistic approximation of $\chi^0$, we have to take into account the structure of the 2-DHG. To this end, the first-order change of the wave functions due to $V(q)$ is calculated by perturbation theory. The result is the well known Lindhard screening\[^5\]:

$$\chi^0(q) = \sum_k \frac{f(k+q) - f(k)}{\epsilon(k+q) - \epsilon(k)}$$

$$= \frac{m^*}{\pi \hbar^2} \left[ 1 - \Theta(q - 2k_F) \sqrt{1 - \frac{4k_F^2}{q^2}} \right]$$

(4.11)

$$V(q) = \int dz V(q,z)|\phi(z)|^2$$

(4.12)

(4.13)

where $f$ is the Fermi distribution function and $\Theta$ is the step function (see Fig. 4.2). At finite $T$, the density response function depends on the dispersion relation $\epsilon_q$ and the position of the electrochemical potential $\mu$. Here we take $\epsilon_q = \hbar^2 q^2 / 2m^*$ and the density response function is \[^5\]:

$$\chi^0(q) = \frac{m^*}{\pi \hbar^2} \Pi(q,T)$$

(4.14)

$$\Pi(q,T) = \int_0^1 \frac{1}{\exp\left[ \frac{\epsilon_q}{4k_BT} (1 - x^2) - \frac{\mu}{k_BT} \right] + 1}$$

(4.15)

For elastic scattering we always have $q \leq 2k_F$, so that the Thomas-Fermi and the Lindhard screening (at $T = 0$) are equal for this scattering process.
Fig. 4.2: While Thomas–Fermi screening is equally effective at all wave vectors $q$, the more realistic Lindhard screening function shows reduced screening for $q > 2k_F$.

As mentioned, exchange and correlation effects have been neglected in both Thomas-Fermi and Lindhard screening calculations. This shortcoming can be removed by introducing a local field correction $G(q)$ by setting $\chi(q) = [1 - G(q)]\chi^0(q)$. Only two particle correlations are taken into account. The local field correction can then be calculated using the structure factor $S(q)$.

$$G(q) = -\frac{1}{n} \int \frac{d^2q'}{(2\pi)^2} \frac{qq'}{|q||q'|} [S(q - q') - 1] \quad (4.16)$$

which is typically calculated in the Hartree-Fock approximation, yielding

$$G(q) = \frac{1}{2n_\nu} \frac{q}{\sqrt{q^2 + k_F^2}} \quad (4.17)$$

Here, $n_\nu$ denotes the valley degeneracy of the band structure, which is 1 for holes in SiGe.
4.2.2 Dielectric function $\varepsilon$

In the previous section, the density change due to an internal potential was calculated. This potential includes screening effects and is not known a priori. Instead, the unscreened potential $V_0(q)$ is known, for example the unscreened Coulomb potential.

In quasi-2D, in the absence of a scattering potential, we have $\Psi(\mathbf{x}) = \phi(z) \exp(\mathbf{i} \mathbf{k} \mathbf{r}) = |k\rangle$, and the probability distribution is constant in the $x$-$y$ plane. Assuming that the external scattering potential is weak enough, the change of the wave function in $z$-direction can be neglected. Therefore, the $z$-distribution of the probability density remains unchanged, while the in-plane probability distribution is modulated by the additional potential. Then it is possible to factorize the modulation of the probability distribution as follows:

$$\rho(x, z) = f(x) \frac{|\phi(z)|^2}{\rho(z)} \quad \rho(k) = \int dz e^{-ikz} \rho(z). \quad (4.18)$$

Here and in the following, we adopt the following nomenclature: $k \equiv k_z$ and $k = (k_x, k_y)$.

Since the difference between screened potential $V(q,k)$ and the unscreened potential $V_0(q,k)$ is produced by the induced charge distribution, the Poisson equation reads:

$$\frac{\rho(q,k)}{\varepsilon_r \varepsilon_0} = (q^2 + k^2)(V(q,k) - V_0(q,k)). \quad (4.19)$$

On the other hand, the 3-D internal potential $V(q,k)$ interacts with the charge density, changing its energy. Since we assume that the $z$-distribution of the charge density is unchanged by the internal potential, the energy change only depends on $q$, but not on $k$. Thus, the interaction has the form of an effective 2-D potential $V_{\text{eff}}(q)$:

$$V_{\text{eff}}(q) = -e \int dk V(q,k) \rho(-k). \quad (4.20)$$

Since we are in the linear response approximation, the energy change leads to a corresponding density change. Using the nomenclature of (4.18), the 2-dimensional probability density is

$$f(q) = e \chi(q) V_{\text{eff}}(q), \quad (4.21)$$

from which we can restore the full probability density distribution:

$$\rho(q,k) = -e \chi(q) \rho(k) \int dk V(q,k) \rho(-k). \quad (4.22)$$

$^{1}$ we made use of the relation $\int_{-\infty}^{\infty} f(x)g(x) \, dx = \int_{-\infty}^{\infty} \hat{f}(k)\hat{g}(-k) \, dk$
Multiplying eq. 4.19 by $\rho(-k)$ and integrating, we obtain

$$
\int dk V(q, k)\rho(-k) = \int dk V_0(q, k)\rho(-k) - \frac{e^2}{\varepsilon_r \varepsilon_0} \int dk \frac{\rho(k)\rho(-k)}{k^2} \int dk V(q, k)\rho(-k)
$$

$$
V_{\text{eff}}(q) = V_{0,\text{eff}}(q) - \frac{e^2}{\varepsilon_r \varepsilon_0} \int dk \frac{\rho(k)\rho(-k)}{k^2} \chi(q)V_{\text{eff}}(q).
$$

Using the definition of $\rho(k)$, we are able to give $\hat{\nu}(q)$ more meaning:

$$
\hat{\nu}(q) = \int dk \int d\tau \int d\tau' \rho(z)\rho(z')e^{i k(z-z')} = \int d\tau \int d\tau' \rho(z)\rho(z')e^{-q|z-z'|}.
$$

The leading term in (4.26) describes the bare interaction of a true 2-D system [60]. The form factor $F_{\text{scr}}(q)$ describes wave function specific deviation of the interaction potential from a true 2-D system (for which $F_{\text{scr}}(q) = 1$). It is worth noting that the form factor is always smaller than unity since the exponential is always smaller than one. In other words, the spread of the wave function in z-direction reduces the amount of screening the gas can provide.

We now solve for the effective potential $V_{\text{eff}}$. The final result for the effective scattering potential is

$$
V_{\text{eff}}(q) = \frac{1}{1 + \hat{\nu}(q)\chi(q)}V_{0,\text{eff}}(q)
$$

$$
= \frac{V_{0,\text{eff}}(q)}{\varepsilon(q)}
$$

which is the definition of the dielectric function $\varepsilon(q)$.

### 4.3 Scattering mechanisms

#### 4.3.1 Charged impurities

The axes are chosen such that the center of the quantum well is located at $z = 0$. A fixed charge at $z_0$ has an external potential $V'(z, r) = e^2/4\pi\varepsilon\varepsilon_0\sqrt{(z - z_0)^2 + r^2}$. When such
4.3. SCATTERING MECHANISMS

Charges are randomly distributed in a 2-dimensional sheet at position $z_0$ with areal density $N_{2D}$, the scattering matrix element evaluates as

$$\langle k' | V | k \rangle^2 = N_{2D} \left| \int dr e^{i(k' - k) \cdot r} \int_{-\infty}^{\infty} dz |\phi(z)|^2 \frac{V'(q, r)}{\epsilon(q)} \right|^2 = \frac{e^2}{4\pi\epsilon\epsilon_0 q (1 + \tilde{v}(q) \chi(q))} \int_{-\infty}^{\infty} dz |\phi(z)|^2 e^{-2q|z| - z_0} \right|^2 \tag{4.29}$$

$$S(q) = N_{2D} \left( \frac{e^2}{4\pi\epsilon\epsilon_0 q (1 + \tilde{v}(q) \chi(q))} \right)^2 \int_{-\infty}^{\infty} dz |\phi(z)|^2 e^{-2q|z| - z_0} \right|^2 \tag{4.30}$$

where $q = |k' - k|$ is the scattering vector and $S(q)$ is the structure factor as defined in Eq. 4.7. The Coulomb scattering form factor $F_C$ is defined by

$$F_C = \int_{-\infty}^{\infty} dz |\phi(z)|^2 e^{-2q|z| - z_0} \tag{4.31}$$

and describes the influence that the position of the scattering center and the shape of the wave function have on the scattering cross section. If the charge is far away from the gas ($z_0 \gg w$), $F_C$ evaluates to $\exp(-2qz_0)$ (remote impurity scattering). For charges close to or inside the channel, it is necessary to fully take into account the shape of the wave function.

The mobility of the 2DHG increases with carrier density if charged impurities are the main scattering mechanism. Screening by the other electrons removes the pole in the differential scattering cross section at $q = 0$ in eq. 4.29. As the form factor $F_C$ decays with increasing $q$, scattering from charged impurities favors small angle scattering. On the Fermi surface, the forward momentum lost in a collision with momentum transfer $q$ is $\Delta p = k_F(1 - \cos \theta) = q^2 / 2k_F$. This fraction becomes smaller as $k_F$ increases, leading to increased carrier mobility.

When the scattering centers are distributed homogeneously with a volume density $N_{3D}$ instead of being arranged in two narrow sheets, we get

$$S(q) = N_{3D} \left( \frac{e^2}{4\pi\epsilon\epsilon_0 q (1 + \tilde{v}(q) \chi(q))} \right)^2 \int_{-\infty}^{\infty} dz_0 F_C(q, z_0)^2. \tag{4.32}$$

Due to screening by the gas, $S(q)$ does not have a pole at $q = 0$ when the charges are arranged in a 2D sheet, which can be seen by inserting the expression for $\tilde{v}(q)$ (eq. 4.26). On the other hand, for homogeneously distributed charges it does have a simple pole at $q = 0$, coming from the integral in eq. 4.32. This means that the quantum scattering rate
Chapter 4. MOBILITY

(eq. 4.10) becomes infinitely large in this approximation. The quantum scattering time remains finite if the $z_0$-integration is not carried to infinity, i.e., by introducing a cutoff. As the divergence is slow (logarithmic), one can even use the physical thickness of the sample as integration limit. For the samples discussed below, this would result in Dingle ratios $\alpha$ of about 20-30.

For both geometries, the transport scattering lifetime is finite. The Dingle ratio can thus be calculated directly for a 2-dimensional sheet. For a homogeneous distribution, it can only be calculated if either volume screening is known or a cutoff is introduced, but in any case it can be expected that the Dingle ratio should be about 20-30 in high mobility SiGe/Ge heterostructures.

4.3.2 Short range scattering

Short range scattering is characterized by an exponential decay of the autocorrelation function of the scattering potential. The bare scattering potential can be calculated directly from the Fourier transform of the autocorrelation function of the scattering potential:

$$\int dr e^{-iqr} \langle V(x + r) V(x) \rangle_x = \int dr e^{-iqr} \int dx V(x + r) V(x)$$

$$= \int dr e^{-iqr} \int dk \int dk' \int dxe^{ik(x+r)} e^{ik'x} V(k) V(k')$$

$$= \int dk \int dk' e^{ikr} V(k) V(k') \delta(k + k')$$

$$= \int dk V(k)V(-k) \int dr e^{-iqr} e^{ikr}$$

$$= V(q)V(-q) = |V(q)|^2$$

(4.33)

The usual example for short range scattering is interface scattering, i.e. scattering from a rough channel-cladding interface for which it is customary to assume \[55\] that $|V(q)|^2 = \Delta^2 \Lambda^2 \exp[-\Lambda^2 q^2]$. In this treatment all properties of the scattering potential have been reduced to an amplitude $\Delta$ and a correlation length $\Lambda$. In particular, the shape of the wave function and the $z$-dependence of the scattering potential is lumped into $\Delta$. Consequently, the origin of the scattering does not have to be located at the interface, but can be anywhere inside or in the vicinity of the channel. For example, potential fluctuation associated with point defects cannot be distinguished from scattering due to channel interface roughness. Thus, the observation of short range scattering does not necessarily indicate a rough interface, but can have other origins, as will be shown below.
4.4 Experimental results

4.4.1 Frontside doped samples

To investigate the limiting mechanisms for hole mobility, a range of samples with similar geometry was grown with the doping between the channel and the sample surface, as shown in the right panel of Figure 4.1. All samples have a virtual substrate with a final Ge concentration of 70%, a cladding of the same composition, but grown at reduced rate and temperature, a 17 nm wide well, a 10 nm spacer, a single boron δ-doping, a 20 nm thick cover layer and are finally covered with 2-3 nm of Si to make the surface more environmentally stable.

The samples differ significantly in the actual carrier density, despite the fact that they were all doped according to the same recipe. The cause is not precisely known, but it is likely that the amount of precursor gas was not the same every time. The precursor diborane (B$_2$H$_6$) is a relatively instable compound and is used in dilute form (100 ppm in argon). To overcome decay effects of the precursor the gas line is emptied through the growth chamber and refilled before the growth of the sample is started. The doping time is so short that only the most forward part of the gas line content is actually used, and its diborane content will determine the sample sheet carrier density.

The choice of the location on the wafer where the sample is taken from is crucial: the growth system shows strongly non-uniform growth rates. Although most of the layer thickness variations are probably due to non-uniform plasma density, the sample temperature is also not absolutely uniform over the sample. Therefore, to make useful statements about sample properties, the samples have to be taken from the same spot on their wafers. This is simplified somewhat by the fact that (001) silicon can only be cleaved in the two (110) directions. As the primary flat is taken as the reference, the sample location is highly reproducible.

Figure 4.3 shows the mobility of pieces taken from the area with the highest growth rates, which also happens to be the area with the highest mobility. Individual samples (cleaved squares) are indicated by red triangles. The resistance of these samples was measured in a van der Pauw geometry with soldered indium contacts at the corners. Sometimes, the same sample accounts for two or three points in the graph. In that case, the carrier density was varied by using a different cooling rate from room temperature down to 2.0 K, where all the mobility measurements were performed. This behavior is presumably related to different freeze-out of charges, particularly charges at the sample surface.

Data from individual squares is complemented by data from two gated Hall bar samples,
Fig. 4.3: The mobility of Ge/Si$_{0.3}$Ge$_{0.7}$ heterostructures [52] can be described as being limited by interface charges. An interface impurity density $N = 4 \times 10^{10}$ cm$^{-2}$ best matches experimental results. Both individual, ungated samples (▲) and gated samples (♦, •) follow the same relation. A density dependent effective mass $m^*$ has been taken into account [54]. The mobility can be seen to fall below the fit for densities below $2 \times 10^{11}$ cm$^{-2}$, and samples do not conduct when the density falls below $1 \times 10^{11}$ cm$^{-2}$, which indicates a metal-insulator transition in our samples, probably driven by carrier density fluctuations (percolation transition).

shown in Fig. 4.3 as magenta circles and blue diamonds. It extends the available data to low sheet carrier densities. Moreover, it also coincides with the mobility of individual samples at high density. As the carrier density is reduced below $2.5 \times 10^{11}$ cm$^{-2}$, the mobility bends down and seems to tend toward zero at $p_s = 1.0 \times 10^{11}$ cm$^{-2}$. This behavior is
not unexpected, since reduced mobility impairs screening, leading to a threshold below which the mobility can only be zero. However, this mechanism becomes important only for sheet resistances of the order of $h/e^2$, which would be reached at a carrier density of $5 \times 10^{10} \text{cm}^{-2}$. As the extrapolated zero mobility point has significantly higher carrier density, it is likely that a different mechanism is responsible for the bending of the mobility curve.

A possible candidate would be a macroscopic carrier density fluctuation leading to a percolation transition. This means that the fluctuating background potential leads to local carrier density modulations. When the carrier density is decreased, patches with $p_s = 0$ will evolve until finally the regions with non-vanishing carrier density will no longer be connected and the sample becomes an insulator.

Both gated samples were fabricated from wafer 7158. They are standard hall bars and SiO$_2$ was used as gate dielectric.

The mobility of individual samples is clearly spread around a line with the mobility roughly proportional to the sheet carrier density. This behavior is typical for charged impurity scattering, in which small angle scattering events dominate. As a result, the average scattering angle decreases with carrier density, as does the average momentum loss.

To calculate the theoretical mobility, the wave function is modeled by a product of a cosine and an exponential function, allowing for an analytic treatment of the form factors while preserving the key features such as the center position and the width of the wave function. In particular, the wave function can model different electric fields at the interface. This interface field depends on the carrier density. The following formula is used for the probability density inside the well:

$$\rho(z) = \frac{(\alpha^2 + \pi^2)}{(1 + e^{\alpha}) L \pi} \cos \left( \frac{\pi z}{L} \right) \exp \left[ -\alpha \left( z - \frac{L}{2} \right) \right]. \quad (4.34)$$

Outside the well, $\rho(z) = 0$. Please note that the use of a simple cos function is not a typing error. From square well potentials, one might expect a cos$^2$ here, but the density function used fits the results of the band structure calculation much better. The value of the parameter $\alpha$ allows to tune the shape of the wave function. Zero would be used for a symmetric well, while large values of $\alpha$ are used for approximately triangular wells. In particular, $\alpha$ is a function of the carrier density and was varied as a function of $p_s$ when calculating the mobility, in accordance with results of the band structure calculations.

As it will become important in the following, we introduce interface charge scattering here. It is a special case of scattering from a 2-dimensional sheet of carriers. There are two such sheets, one at each channel interface, which are at position $z_1$. The scattering
rate \( w = 1/\tau_{tr} \) from one interface is calculated as

\[
w = \frac{N_{imp} m}{2\pi \hbar^3 k_F} \left( \frac{e^2}{2\epsilon\epsilon_0} \right)^2 \int_0^{2k_F} \left( q + F_{self}(1-G)q_s \right)^2 \frac{dq}{2k_F^2} \frac{dq}{\sqrt{1 - \frac{q^2}{4k_F^2}}} \tag{4.35}
\]

\[
F_{self} = \int \int d\bar{z} d\bar{z}' \rho(\bar{z}) \rho(\bar{z}') e^{-q|\bar{z} - \bar{z}'|} \tag{4.36}
\]

\[
F_{IC} = \int |\phi(z)|^2 e^{-q|z-z_I|} \tag{4.37}
\]

where \( z_I = \pm L/2 \) denotes the position of the heterointerface. The parameter \( a \) is chosen to get the best match to the result of a band structure calculation.

Calculations of the quantum scattering time and the Dingle ratio are straightforward. For a sheet carrier density above \( 4 \times 10^{11} \text{ cm}^{-2} \), the Dingle ratio has a value between 5 and 6. The experimental determination of the Dingle ratio is subject to error of order unity.

Charged interface impurity scattering is sufficient to explain the observed data. However, it has to be noted that scattering from interface impurities cannot reliably be distinguished from homogeneously distributed charged impurities by mobility measurements alone (the reasons that rule out homogeneous impurity scattering will be discussed later). The scattering cross section of charged impurities vanishes exponentially with increasing distance from the channel, making scattering a very local property (in \( z \)-direction). Therefore, a homogeneous distribution effectively acts like a finite slab of scatterers, and the carrier density dependence is almost like that of a narrow sheet of charge located at either interface. In fact, cutting off the \( \tau_{tr} \) \( z_0 \)-integral at a distance of 15 nm either side of the channel does not noticeably alter the result of the calculation. This is of course not true for the calculation of \( \tau_q \), where one can argue what cutoff to use to avoid divergence of the integral. Anyway, the physical thickness of the sample sets an upper limit for the cutoff, and the Dingle ratio will not exceed 25 for a cutoff of 100 \( \mu \)m, and even a cutoff of 1 mm (which is twice the thickness of the sample) only leads to a maximum \( \alpha = 27 \). Dingle ratios close to the experimental ones are found for a cutoff of 2 \( \mu \)m.

From the above it is clear that a combination of interface and homogeneous charge can be used to get almost any Dingle ratio between 5 and 25. This also explains the spread from sample to sample that is observed experimentally.

Additional observations are in favor of the predominance of interface impurity scattering. Explaining the experiments by homogeneously distributed charges requires an impurity density around \( 4.5 \times 10^{16} \text{ cm}^{-3} \). As one would have to assume the same impurity density throughout the virtual substrate, the room temperature resistance would always be less than 100 \( \Omega \). Since this is not observed, we conclude that homogeneous impurities alone
cannot account for the observed mobility. Concerning the importance of remote impurity scattering from the doping layer, we observe that increasing the spacer width to 20 nm did not show a significant change in mobility. Even the large spacer width of 40 nm, used in the inverted p-MOD 7404 and in the double sided p-MODs 7319 and 7396, did not lead to the increase in mobility that would be expected if remote impurity scattering was dominant.

A different explanation of the experimental mobility was set forth in [52]. The paper ascribes the observed mobility to a combination of interface impurity and remote impurity scattering. The quality of the fit is equal to that of the scattering mechanism proposed in this work. However, further experiments have made the explanation of [52] less likely than the one proposed in this work. In particular, the mentioned insensitivity of the experimental mobility to the variation of the spacer width makes a dominance of remote impurity scattering questionable. Moreover, to reduce the calculated Dingle ratios to the ones observed experimentally, spatial correlation of the remote charges had to be assumed, as detailed in [64]. The idea is that if the remote charge layer is only partially ionized, the mutual Coulomb interaction will try to maximize the average distance between ionized centers, introducing correlation into the random arrangement of centers that is created during growth. Of course, this requires the energy of the charge layer to match the Fermi energy.

The interpretation set forth here is more consistent with observations in that here the spacer width does not play a role and no charge correlation is required to explain the observed Dingle ratios. This shows that the relatively large number of possible scattering mechanisms typically allows for different explanations of a given observation.

4.4.2 The backside doped sample 7404

Originally this sample was grown to explore the feasibility of backside doped structures (Figure 4.1, left panel). The issue here is that not all dopant atoms are incorporated into the sample, but segregate (“float” on the growing surface), while gradually being incorporated into the lattice. This process introduces charged impurities into the channel, impairing mobility. Attempting to limit the consequences of segregation, the spacer was increased to the maximum width compatible with the intended carrier density ($4 \times 10^{11}$ cm$^{-2}$). Due to the doping arrangement, the wave function is expected to sit close to the lower interface rather than the upper, which is the case with front side doped samples.

The experimental result shown in Fig. 4.4 exceeds all expectations: Especially at carrier
**Fig. 4.4:** The mobility of sample 7404 (symbols) can be explained by the interplay of local charge scattering (dash-dotted line) and short range scattering (dashed line). The total mobility (solid line) shows an increase almost proportional to the density below $4 \times 10^{11}$ cm$^{-2}$, then gradually turning over as short range scattering becomes more important at higher density. Two devices made from the backside doped sample 7404 are shown, 7404-12 is shown as-cooled (red circles) and after illumination (magenta diamonds), 7404-15 was only measured in an illuminated state (blue triangles).

Densities below $4 \times 10^{11}$ cm$^{-2}$, the mobility is higher than in any front side doped sample in literature. In this regime, the observed mobility can be explained again by interface charge scattering, using a density of $2.4 \times 10^{10}$ cm$^{-2}$. This number is noticeably lower than that found for front side doped samples. The thought that the lower interface of a backside doped structure contains fewer interface charges than the upper interface of a
front side doped structure sounds counterintuitive at first, since at the time of channel deposition the front side structure is virtually undoped. However, one has to keep in mind that from a growth point of view the two surfaces are different. When the channel starts to grow and the lower interface is formed, the substrate is unstrained and flat. During the deposition of the channel, the surface of the sample starts to roughen due to the compressive strain. The growth of the upper cladding then takes place on an undulated strained surface. Therefore, the number of charged defects that form at either interface during growth may be different. As the 2DHG sits close to the dopant side of the channel, it will feel a different impurity density for normal and inverted doping.

As mentioned, mobility measurements cannot distinguish between charges localized at the interface and homogeneously distributed charges. Either way it is obvious that the scattering centers have not been introduced by the doping procedure.

As the carrier density is increased beyond about $4 \times 10^{11}$ cm$^{-2}$, the mobility increase slows down and the mobility eventually becomes approximately independent of carrier density. This behavior is a clear indication of short range scattering. The experiment can be explained by a short range scattering with a correlation length $\Lambda = 1.5$ nm and a scattering amplitude of 4 meV.

![Image](image.png)

**Fig. 4.5:** Cross section Transmission Electro Microscopy reveals the source of short range scattering in sample 7404: point defects locally distort the crystal lattice. The size of the distortion is about 2 nm, matching well with the correlation length of 1.5 nm deduced from transport experiments.

Short range scattering is usually associated with short ranged roughness correlations in
the interface between channel and cladding. As cross section Transmission Electron Microscopy (TEM) images show, the lower interface is usually flatter than the upper interface, which is a consequence of the compressive strain in the channel that leads to roughening during growth. Therefore, one would expect a larger contribution from interface roughness when the wave function is located close to the upper interface. This is the case if the doping layer is above the channel. Since the front side doped samples show an ever increasing mobility with carrier density (Fig. 4.3), interface roughness is obviously no issue with these samples, and should not be with backside doped samples either. The observation of short range scattering was therefore very intriguing.

Cross section TEM images of the backside doped sample (Fig. 4.5) reveal that the interface quality is indeed excellent. The true reason for short range scattering is also apparent: The high resolution TEM image has a speckled appearance. These speckles exist due to lattice distortions, changing the contrast of the TEM image. The distortions are due to point defects. Their nature is unclear, but vacancies or silicon / germanium interstitials can be excluded. These types of point defects should vanish when the sample is annealed at sufficient temperature, which is not the case. It is therefore most probable that the contrast is due to foreign atoms sitting on lattice sites.

TEM images also suggest that the distribution of defects is not homogeneous. Density variations between individual images suggest that the distribution can vary over distances as low as 1 mm. Therefore, a certain variation from Hall bar to Hall bar is expected, explaining the difference of 7404-15 and 7404-12.

Since the occurrence of short range scattering is not observed in typical samples, further improvement of the mobility of backside doped samples can be expected. Especially at carrier densities above $4 \times 10^{11}$ cm$^{-2}$, the possible improvement is large, and it is very well possible that in the future the samples with the highest mobility are doped underneath the channel.
Chapter 5

Magnetoresistance

In the simplest theoretical model of metallic conduction developed by Drude, assuming a constant scattering time \( \tau \) and a Fermi surface with constant effective mass \( m^* \), the conductivity in a magnetic field is found to be

\[
\sigma = \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} \\ \sigma_{xy} & \sigma_{xx} \end{pmatrix}
\]

\[
= \frac{\sigma_0}{1 + \mu^2 B^2} \begin{pmatrix} 1 & -\mu B \\ \mu B & 1 \end{pmatrix}
\]

\[
\sigma_0 = e\mu n, \quad \mu = \frac{e\tau}{m^*}
\]

(5.1)

(5.2)

(5.3)

where \( n \) is the carrier density. Inversion of the conductivity tensor shows that the longitudinal resistance \( \rho_{xx} \) is independent of the magnetic field \( B \):

\[
\rho = \begin{pmatrix} \rho_0 & R_H B \\ -R_H B & \rho_0 \end{pmatrix}
\]

\[
\rho_0 = \sigma_0^{-1}, \quad R_H = \frac{1}{ne}
\]

(5.4)

(5.5)

To explain magnetic field dependent resistance in classically weak magnetic fields (\( \mu B \ll 1 \)), a number of corrections to the Drude result exist.

When the current is carried by more than one species of carriers, i.e. if the scattering time \( \tau \) can not be assumed to be constant but the Fermi surface is still elliptic, the resistance in a magnetic field \( B \neq 0 \) is always larger than without the field (positive magnetoresistance). The reconstruction of an assumed distribution \( n(\mu) \) of carriers with a certain mobility \( \mu \) is the goal of the so called mobility spectrum analysis (MSA) [65–67]. However, the technique requires numeric inversion of an integral transform which is ill
conditioned. Several methods have been proposed to perform the task and work well on artificial data. Fed with experimental data, the calculations have a tendency to produce unrealistic artifacts, which may be due to the fact that the underlying model does not capture the whole physics. In particular, a magnetic field dependent scattering time is excluded by the model.

When the Fermi surface is no longer described by an ellipsoid, the cyclotron motion of a carrier in a magnetic field becomes more complicated, giving rise to another form of positive magnetoresistance which will be treated in the next section.

Negative magnetoresistance (NMR), i.e. the resistance in a magnetic field \( B \) is smaller than without the field, is found as a consequence of quantum interference (weak localization) and electron-electron interaction.

There is also a semiclassical effect that produces NMR [68–70]. It is caused by the trapping of carriers onto stationary orbits around scattering centers. Since the mechanism requires that a carrier can complete a cyclotron orbit, “enabling” it to collide with the same scatterer again and again, a classically strong magnetic field is required (\( \mu B \gg 1 \)).

### 5.1 Band structure induced magnetoresistance

The simple Drude theory of metallic conductivity predicts the longitudinal resistance \( \rho_{xx} \) to be independent of a magnetic field \( B \). As has been shown by McClure [71], this is due to the assumption of an ellipsoidal Fermi surface and a constant scattering time. With these restrictions relaxed, the resistance can become field dependent. The hole bands of germanium rich SiGe alloys are far from being ellipsoidal.

Throughout this section, vectors and matrices are typeset in boldface (e.g. \( \mathbf{k} \)) and scalars are typeset normal (e.g. \( k = |\mathbf{k}| \)).

#### 5.1.1 McClure’s approach

In this section the results of McClure [71] are repeated in part, adapted to the 2-D case with a magnetic field perpendicular to the transport plane.

The basic assumption is that there is a relaxation time \( \tau \), which may depend on \( \mathbf{k} \). The particle distribution function \( f \) is written as \( f = f_0 + \phi \partial f_0 / \partial E \), where \( f_0 \) is the equilibrium distribution function in absence of a current and \( E \) is energy. To first order in the electric...
field $\mathcal{E}$, the Boltzmann transport equation can be written as

$$\frac{\partial \phi(s)}{\partial s} + \frac{\phi(s)}{\tau(s)} + e\mathcal{E} \cdot \mathbf{v}(s) = 0 \quad (5.6)$$

where $s$ parametrizes a constant energy surface $\Gamma$ such that

$$\frac{\partial \mathbf{k}}{\partial s} = -\frac{e}{\hbar} \mathbf{v} \times \mathbf{B}. \quad (5.7)$$

It is obvious that $s$ is just the time and that equation (5.6) is periodic with a cycle duration $T = 2\pi/\omega_c$, where $\omega_c = eB/m^*$ is the cyclotron frequency and $m^*$ is the DOS mass on the surface $\Gamma$.

The general solution to equation (5.6) is

$$\phi = -\int_{-\infty}^{s} ds' e\mathcal{E} \cdot \mathbf{v}(s') \exp \left[-\int_{s'}^{s} ds''/\tau(s'')\right] \quad (5.8)$$

Expanding $\mathbf{v}$ into a Fourier series, $\mathbf{v}(s) = \sum_{-\infty}^{\infty} \mathbf{v}(m) \exp[i\omega_c ms]$ and assuming $\tau$ to be independent of $s$, the conductivity can be calculated as

$$\sigma = -\frac{e^2}{(2\pi)^2} \int d^2k \frac{\partial f_0}{\partial E} S \quad (5.9)$$

$$S_{xx} = \sum_{m=1}^{\infty} \frac{2|v_x(m)|^2}{1 + (m\omega_c\tau)^2} \quad (5.10)$$

$$S_{xy} = \sum_{m=1}^{\infty} \left\{ \frac{v_x(m)v_y(-m) + v_x(-m)v_y(m)}{1 + (m\omega_c\tau)^2} \right. +$$

$$\left. + i \frac{[v_x(-m)v_y(m) - v_x(m)v_y(-m)]m\omega_c\tau}{1 + (m\omega_c\tau)^2} \right\}. \quad (5.11)$$

Before embarking on how to calculate the band structure induced magnetoresistance, let us first give some of McClure’s conclusions from the general form of equations (5.9), (5.11)

For elliptical Fermi surfaces, all harmonics of $v(m)$ vanish, except the $m = 1$ term. Then the Drude result is recovered, i.e. $\rho_{xx}$ is field independent.

For strained germanium as in our samples, the Fermi surface has inversion symmetry, in accordance with lattice symmetry. Therefore, $\mathbf{v}(s) = -\mathbf{v}(s + T/2)$ and all even Fourier components of $v(m)$ vanish.

Exploiting lattice symmetry a little more, we also see that $v_y(m) = \pm iv_x(m)$. The sign determines the sign of the Hall effect and hence distinguishes hole and electron transport. Since $\mathbf{v}(t) \in \mathbb{R}$ we also have $\mathbf{v}(-m) = \overline{\mathbf{v}(m)}$. Inserting this into equation (5.11), we find

$$S_{xy} = \pm \sum_{m=1}^{\infty} \frac{2|v_x(m)|^2 m\omega_c\tau}{1 + (m\omega_c\tau)^2} \quad (5.12)$$
5.1.2 Calculation of magnetoresistance, constant $\tau$

The work of McClure does not attempt to calculate specific coefficients $v(m)$ since it was not possible at the time. Using our band structure calculations of chapter 3, we now set out to calculate the expected magnetoresistance. To this end it is obviously necessary to find the cyclotron orbits in $k$ space, which are also constant energy surfaces, and the group velocity of the holes along this surface. Since the band structure calculation gives the energy as function of $k$, the constant energy surfaces have to be interpolated by suitable means as shown below.

![Figure 5.1: Approximation of a constant energy surface: the results of a band structure calculation (black crosses) are interpolated radially (green lines) to find points of the constant energy surface (red and blue points). These are then used as knots for a periodic interpolating spline (red and blue line). Rashba splitting lifts the degeneracy of the spin directions (red and blue line), particularly in the $\langle110\rangle$ directions. Consequently, there are two different constant energy surfaces for the different spin directions.]
We start with a part of our calculated band structure, which is typically given by a set $k_i$ and the corresponding energies $\epsilon_i$, as shown in Fig. 5.1. Typically, the $k_i$ form a square grid or a radial grid. In the following, we will assume that we deal with a radial grid such that there is a set of angles $\phi_i$ and a set of $k_j$. This is the way a band is calculated in chapter 3. We then have $\epsilon_{ij} = \epsilon(k_x, k_y) = \epsilon(k_j \cos \phi_i, k_j \sin \phi_i)$.

We first have to find an approximation to the constant energy surface $\Gamma$ with $\epsilon(\Gamma) = \tilde{\epsilon}$. As a start, it is convenient to choose the angle $\phi$ as curve parameter. The surface $\Gamma$ is then completely specified by the function $k_{\Gamma}(\phi)$, which gives the magnitude of the wave vector that fulfills $\epsilon(k_{\Gamma}(\phi), \phi) = \tilde{\epsilon}$ for a given angle $\phi$. Examples for $k_{\Gamma}(\phi)$ can be seen in Fig. 5.1, where they are shown for the two spin-split heavy hole bands at an energy of 40 meV above the band edge. For every $\phi_i$, the value of $\tilde{k}_i$ with $\epsilon(\tilde{k}_j \cos \phi_i, \tilde{k}_i \sin \phi_i) = \tilde{\epsilon}$ is determined by a suitable interpolation of the corresponding $\epsilon_{ij}$. Then, the function $k_{\Gamma}(\phi)$ is approximated by forming a periodic spine with the sets $\phi_i$ and $\tilde{k}_i$.

\[ \frac{\epsilon}{\partial k} = \text{const} \]

\[ k = \text{const} \]

\[ x \]

\[ \alpha \]

\[ k \]

\[ \phi \]

\[ \epsilon = \text{const} \]

\[ k \partial k \]

\[ \epsilon \partial k \]

\[ \epsilon \partial k \]

\[ \alpha \]

\[ v \]

\[ d\epsilon/dk \]

\[ d\epsilon/k \]

\[ \frac{1}{h} \frac{\partial k}{\partial \phi} \]

\[ \text{Fig. 5.2: To calculate the group velocity } v = \nabla_k \epsilon \text{ from the easily accessible } d\epsilon/dk, \text{ the angle } \alpha \text{ between constant energy surfaces and constant } k\text{-surfaces has to be calculated.} \]

The group velocity $v = 1/h \nabla_k \epsilon$ is found in a similar way. The slope of $\epsilon$ along a radial is easily found. To obtain the absolute value of $v$, we resort to the fact that $\Gamma$ and $v$ are perpendicular. We first calculate the angle $\alpha$ between a radial and $\Gamma$ using the relation (see also Figure 5.2)

\[ \tan \alpha = -\frac{1}{h} \frac{\partial k}{\partial \phi}. \]  

(5.13)
From this we obtain

$$|\mathbf{v}| = \frac{1}{\cos \alpha} \frac{\partial \epsilon}{\partial k}$$

(5.14)

$$v_x = |\mathbf{v}| \cos (\phi - \alpha).$$

(5.15)

In practice, the group velocity is determined only on the knots $\tilde{k}_i$ and again interpolated with a periodic spline. The spline $v(\phi)$ parametrizes the magnitude of the group velocity, while $v_x(\phi)$ parametrizes its component along the x-axis.

\[\text{Fig. 5.3: The magnetoresistance calculated from the band warping using the parameters for sample 6842-1a-51 show that the magnitude of the magnetoresistance as well as the shape is well reproduced by theory. The magnitude of the theoretical prediction is slightly lower than the measured magnetoresistance, shown in Fig. 5.5. The magnetic field scale, however, is scaled by a factor of } \approx 5 \]
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Integration is performed by interpolation with a periodic spline and subsequent symbolic integration. The relation \( s(2\pi) = T = 2\pi/\omega_c = 2\pi m^*/e|B| \) provides a nice way of comparing the calculation with experimental results.

The final step is the calculation of \( v_x(m) \), using the equation

\[
\begin{align*}
v_x(m) & = \frac{1}{T} \int_0^T v_x(\phi(s)) e^{-im\omega_c s(\phi)} ds \\
& = \frac{1}{T} \int_0^{2\pi} v_x(\phi) e^{-im\omega_c s(\phi)} \frac{ds}{d\phi} d\phi \\
& = \int_0^{2\pi} v_x(\phi) e^{-im\omega_c s(\phi)} \left| \frac{1}{|v|} \frac{dk}{d\phi} \right| d\phi \left/ \int_0^{2\pi} \left| \frac{1}{|v|} \frac{dk}{d\phi} \right| d\phi \right).
\end{align*}
\]

Again, the integrands are defined only on the knots \( \tilde{k}_i \) and used to interpolate with a periodic spline, which is then integrated symbolically. The calculation of \( S_{xx} \) and \( S_{xy} \) is straightforward.

After using the tensor inversion to obtain the resistivity, the result of the calculation, shown in Fig. 5.3, can be compared to the experimental result (Fig. 5.5). The amplitude is reproduced quite well, together with the shape of the magnetoresistance. The magnetic field scale, however, is off by a factor of about 5. This discrepancy can not be remedied within the model of McClure, since it uses the inverse mobility as a built-in field scale.

5.1.3 Experimental results

In experiments, the band structure induced magnetoresistance is often overlaid by other magnetoresistive effects like weak localization, electron-electron interaction and Shubnikov–de Haas oscillations. Nevertheless, the effect can be observed at any carrier density and independent of sample geometry.

On inspection of (5.10) and (5.12), it is easy to see that the effect should exist only in the range \( \mu B < 1 \), which ranges between 0.1 and 0.3 T in our samples. In contradiction to these predictions, the effect prevails at significantly higher magnetic field strengths, especially at high carrier density, which is usually accompanied by high carrier mobility. The mobility of the van der Pauw square 6777-2 in Fig. 5.4 is 7.6 T\(^{-1}\) at a carrier density \( n_s = 5.9 \times 10^{11} \text{ cm}^{-2} \), setting the characteristic field for the positive magnetoresistance at 0.15 T. In the experiment, positive magnetoresistance can be seen to prevail at fields up to 0.4 T.

From equations (5.10) and (5.12), one would further expect the resistance to become field independent when \( \mu B \gg 1 \), which is not observed experimentally. Figure 5.4 shows
Fig. 5.4: The band structure induced magnetoresistance of sample 6777-2 is overlaid with the effects of electron-electron interaction. The positive magnetoresistance around $B=0$, visible in all curves, is the result of the band structure induced magnetoresistance. At $B = 0$, the resistance falls as the temperature rises from 1.9 K to 4.9 K in steps of 0.5 K. This temperature dependent resistance is due to electron-electron interaction. The inset shows the magnetoresistance spectrum at 1.9 K, where a pronounced oscillation of the SdH minima can be observed. Among the possible explanations are beatings of the SdH oscillations or the occupation of a second subband. The latter would help explaining the low-field magnetoresistance. However, this should also be accompanied by reduced mobility, which is not the case.

that the resistance does not become constant as the field is increased beyond 0.3 T. This is due to interaction effects at intermediate fields and finally due to the formation of Landau levels as the magnetic field exceeds 1 T. Although the increased width of the Fermi distribution precludes the observation of Shubnikov–de Haas oscillations at the highest temperatures, Landau levels do form and govern the charge transport. Therefore the semiclassical approach, using the zero-field band structure, is unable to reproduce the
Fig. 5.5: The band structure induced magnetoresistance shows up as positive magnetoresistance at $|B| < 0.4$ T for sample 6843-1a-51. Surprisingly, no temperature dependent effects are present in this field range. As with sample 6777-2 shown in Fig. 5.4, the SdH oscillations show a modulation, particularly of the minima. Here, the mobility is even higher, so that it seems unlikely that a second subband has been occupied. However, no satisfactory explanation can be given for the observed modulation.

An example of a hall bar showing band structure magnetoresistance is sample 6843-1a-51, shown in Fig. 5.5. In contrast to sample 6777-2 show in Fig. 5.4, interaction effects are almost absent in the regime of $|B| < 0.5$ T. Although the effects of electron-electron interaction are expected to diminish with increasing sample conductivity (and thus, for our samples, with increasing carrier density), this absence is unexpected, and we have no explanation for this fact.

Geometric magnetoresistance, i.e. magnetoresistance due to the finite size of the contact metalization, can be ruled out since the effect is too small for the geometries used. The effect leads to an increase of the resistance with magnetic field and shows no saturation.
Calculations show that for van der Pauw squares with triangular contacts covering 10% of the length of a square side each, the relative resistance change between $B = 0$ and $\mu B = 1$ is a mere $10^{-3}$. For Hall bars with the metalization at the end of voltage probes as used in experiment, the effect is even smaller, about $10^{-5}$.

As band warping increases with sheet carrier density, the relative magnitude of the positive magnetoresistance increases with carrier density. For sample 6843-51, the effect is about 4.5%, while it is 5% for sample 6777-2, which is the opposite of what would be expected. With a mobility of 9.8 T$^{-1}$ at a carrier density of $7.6 \times 10^{11}$ cm$^{-2}$, one would expect the positive magnetoresistance of sample 6843-51 to be limited to fields smaller than 0.1 T (Fig. 5.3), which is clearly not the case. Since the field scale is built into the model, there is no straightforward way to correct this discrepancy.

The approach of McClure can explain existence and shape of the positive magnetoresistance at small magnetic fields, and it correctly describes its relative size $\Delta \rho/\rho$. The theory fails to predict the correct magnetic field scale, where the effect prevails out to $B = 5\mu^{-1}$.

At least for samples with relatively high carrier density, like 6777-2 and 6853-1a-51, magnetoresistive effects could have a different origin. If additional subbands are occupied by holes, the Hall voltage cannot balance the Lorentz force on carriers in both subbands simultaneously. The conductivities of the two different subbands have to be added before the conductivity tensor is inverted to give the resistivity. When the mobility of the two subbands is not equal, the longitudinal resistance acquires a positive magnetoresistance.

Another consequence of occupation of a second subband with a low carrier density would result in the modulation of the Shubnikov–de Haas oscillations. This effect can be seen in the insets of Fig. 5.4 and Fig. 5.5. Speaking against the occupation of a second subband is the very high mobility of both samples, while the expectation is that the occupation of a second subband increases the scattering, reducing the mobility. It should be mentioned here that there are other effects like beatings of the SdH oscillations, associated with the spin-split first subband, can also lead to modulation of the SdH oscillations.

### 5.2 Weak localization

Weak localization [72, 73] in two dimensions in the presence of spin-orbit (SO) and magnetic impurity (spin) scattering can be described by [72, 74]
\begin{align*}
\Delta \sigma &= -\frac{e^2}{2\pi^2c^2} \left( \Psi \left( \frac{1}{2} + \frac{B_1}{B} \right) - \frac{3}{2} \Psi \left( \frac{1}{2} + \frac{B_2}{B} \right) + \frac{1}{2} \Psi \left( \frac{1}{2} + \frac{B_3}{B} \right) \right) \quad (5.22) \\
B_1 &= B_{tr} + B_{so} + B_s \quad (5.23) \\
B_2 &= \frac{4}{3} B_{so} + \frac{2}{3} B_s + B_\phi \quad (5.24) \\
B_3 &= 2B_s + B_\phi \quad (5.25) \\
B_x &= \frac{\hbar}{4eD_0\tau_x}, \text{ where } x = tr, so, s, \phi \quad (5.26)
\end{align*}

The spin-orbit contribution to weak localization permits \textit{positive magnetoresistance} or weak \textit{antilocalization}, if the “ordinary” dephasing time $\tau_\phi$ is sufficiently long. The spin term $B_s$ on the other hand suppresses weak localization. In particular, it leads to a saturation of the weak localization effect when the spin scattering time $\tau_s$ is the shortest phase breaking time in the system. This is likely to happen at sufficiently low temperature, since other mechanisms for phase breaking usually vanish with decreasing temperature. Electron-electron interaction has $\tau_{e-e} \propto T^{-2}$ while electron-phonon interaction has $\tau_{e-ph} \propto T^{-2\ldots-4}$, depending on the temperature regime and phonon type (longitudinal or transversal).

### 5.2.1 Electron–phonon dephasing

The electron-phonon dephasing time is given by Rammer\textsuperscript{[75]} as

\begin{align*}
\frac{1}{\tau_{\phi,L}} &= \begin{cases} 
\frac{7\pi\zeta(3)}{12} \frac{(k_BT)^3}{m m c_L^3} & \text{ if } \frac{h c L}{l} \ll k_BT \ll h c_L k_D \\
\frac{\pi^2}{30} \frac{i (k_BT)^4}{m c_L^4} & \text{ if } k_BT \ll h c_L / l 
\end{cases} \\
\frac{1}{\tau_{\phi,T}} &= \begin{cases} 
\frac{\pi^2}{20} \frac{(k_BT)^2}{m c_L^2} & \text{ if } \frac{h c T}{l} \ll k_BT \ll h c_T k_D \\
\frac{\pi^4}{30} \frac{(k_BT)^4}{m c_L^4} & \text{ if } k_BT \ll h c_T / l 
\end{cases} \quad (5.27) \quad (5.28)
\end{align*}

Here, $l$ is the elastic mean free path, the index L (T) denotes longitudinal (transversal) phonons, $m$ is the carrier mass, $M$ denotes the ionic mass, $c$ is the speed of sound, and $\zeta(3) \approx 1.20$. Note that apart from the mean free path $l$, which can be strongly varying from sample to sample, the parameters of the theory can reliably be reproduced with the common growth techniques.

In the low temperature regime, $T \ll h c_{T,L}/(k_B l)$, the elastic mean free path is shorter than the typical phonon wavelength. In the high temperature region, the phonon wavelength is shorter than the elastic mean free path, but the temperature is still below the Debye...
temperature. Since the Debye temperature of Germanium is about 350 K, this is not really a restriction. However, the crossover temperature does depend on the elastic mean free path and has to be considered more carefully. For a typical sample with \( \mu = 6 \text{ m}^2/\text{Vs} \) and \( p_s = 4.5 \times 10^{15} \text{ m}^{-2} \), the elastic mean free path is \( l = 660 \text{ nm} \) and the crossover temperature is \( T_c = 60 \text{ mK} \). As the lowest experimental temperature in this work was 0.4 K, the phonon dephasing rate of this sample should show \( T^{-3} \)-behavior.

5.2.2 electron – electron dephasing

Phase breaking due to electron–electron interaction is easiest to understand if one looks at it as the loss of phase coherence of a single electron due to a time-dependent electric potential created by all the other electrons in the system. The diffusive character of electron motion enhances this effect.

Altshuler et al. \[76\] give the 2-dimensional e-e phase breaking time as

\[
\frac{1}{\tau_\phi} = \frac{e^2 k_B T}{2\pi h^2 \sigma_0} \ln \frac{k_F l}{2}
\] (5.29)

5.2.3 Weak localization - useful formulas

General equations

In the absence of spin-dependent scattering, the weak localization contribution to conductivity can be written as \[72\]

\[
\delta \sigma_{xx}(B) = -\frac{e^2}{2\pi^2 \hbar} \left( \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD \tau_{tr}} \right) - \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD \tau_\phi} \right) \right) - \Psi \left( \frac{1}{2} + \frac{B_{tr}}{B} \right) - \Psi \left( \frac{1}{2} + \frac{B_\phi}{B} \right)
\] (5.30)

where the Digamma function \( \Psi(x) \) is derived from the \( \Gamma \) function (the analytic continuation of the factorial) by

\[
\Psi(x) = \frac{d}{dx} \ln \Gamma(x),
\] (5.32)

the diffusion constant \( D \) can be written as

\[
D = \frac{1}{2} v_F^2 \tau_{tr}
\]

\[
= \frac{k_F^2 k_{Ftr}^2}{2m^*}
\]

\[
= \frac{e_F^2 \tau_{tr}}{m^*}
\]

(5.33)

(5.34)

(5.35)
and the dephasing field $B_{\text{tr}}$ is

$$B_{\text{tr}} = \frac{\hbar}{4eD\tau_{\text{tr}}} = \frac{e^2\rho_0^2}{4\pi\hbar R_H} \quad (5.36)$$

where $\tau$ is the transport scattering time, $\rho_0$ is the resistance at $B = 0$ and $R_H$ is the Hall constant.

**Approximate expressions**

For $B \to \infty$:

$$\frac{e^2}{2\pi^2\hbar} \left( \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD\tau_{\text{tr}}} \right) - \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD\tau_{\phi}} \right) \right) = \frac{e}{16BD} \left( \frac{1}{\tau_{\text{tr}}} - \frac{1}{\tau_{\phi}} \right) \quad (5.37)$$

i.e. the effect of weak localization vanishes only slowly with increasing field. It is inversely proportional to the area per magnetic flux quantum. Of course, the physical effect (not the mathematical approximation!) breaks down if $R_c \gg \ell = v_F\tau$.

For $B \to 0$:

$$\frac{e^2}{2\pi^2\hbar} \left( \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD\tau_{\text{tr}}} \right) - \Psi \left( \frac{1}{2} + \frac{\hbar}{4eBD\tau_{\phi}} \right) \right) = \frac{e^2}{2\pi^2\hbar} \left\{ \ln \frac{\tau_{\phi}}{\tau_{\text{tr}}} - \frac{1}{6} \left( \frac{eBD\tau_{\phi}}{\hbar} \right)^2 + \ldots \right\} \quad (5.40)$$

that is, the amplitude of the weak localization is proportional to $\ln(\tau_{\phi}/\tau)$, the peak shape for small fields is parabolic and its curvature is determined solely by the dephasing time $\tau_{\phi}$.

**5.2.4 Experimental**

Apart from some very low density samples, weak localization is a very tiny effect for the samples used in this study. As shown in (5.22), weak localization is a fixed correction $\Delta \sigma$ to the classical conductivity $\sigma_0$. When measuring resistance in small fields ($\mu B \ll 1$), the resistance change is $\Delta \rho = \rho_0^2 \Delta \sigma$, where $\rho_0 = \sigma_0^{-1}$. In typical samples, the weak localization peak is too low to be measured with the normal setup because the signal is below the noise threshold.

Computing the weak localization of sample 7404-16, with Fermi wave vector $k_F = 1.68 \times 10^8$ m$^{-1}$, mean free path $l = 660$ nm, $\sigma_0 = 4 \times 10^{-3}$ S, effective mass $m^* = 0.085 m_e$, Fermi
velocity $v_F = 2.2 \times 10^5 \text{ m/s}$, transport scattering time $\tau_{tr} = 2.1 \text{ ps}$ derived from the mobility and $\tau_{tr} = 3.3 \text{ ps}$ derived from weak localization yields an electron-electron scattering dephasing time $\tau_{\phi} = 195 \text{ ps}$ at 1.0 K. This time is significantly longer than the time found experimentally. We further compute the diffusion constant $D = v_F^2 \tau_{tr}/2 = 0.079 \text{ m}^2/\text{s}$ and $B_{tr} = \hbar/4eD\tau_{tr} = 0.64 \text{ mT}$.

In Fig. 5.6 we show weak localization measurements and fits to (5.30) for sample 7404-

![Graphs showing weak localization measurements and fits](image)

**Fig. 5.6:** Weak Localization peaks show no signs of weak antilocalization at temperatures down to 0.36 K. Measurements with different excitation currents show no difference in shape and amplitude of the peak. The ratio of the scattering times transport time $\tau_{tr}$ and phase breaking time $\tau_{\phi}$ extracted from a fit to (5.30) are shown in Fig. 5.7.
16. The agreement of fit and data is very good, therefore there is no need to use more complicated formulae like (5.22). The transport scattering time is 3.2 ps and the phase breaking time is 11 ps, significantly shorter than the one computed above for electron interaction dephasing. This means that electron dephasing is significantly enhanced over the theoretical value in these structures. Phonon dephasing can be ruled out as dephasing mechanism, since the phonon dephasing time at 1.0 K is extremely long, on the order of 70 ns for longitudinal and 600 ns for transverse phonons. This mechanism can therefore be ruled out as an effective dephasing mechanism.

![Graph](image)

**Fig. 5.7:** Saturation of the ratio of transport time $\tau_{tr}$ and phase breaking time $\tau_{\phi}$ below 1 K is indicate either a temperature independent dephasing mechanism or failed cooling of the hole gas. Since the ratio shows no current dependence, heating by the measurement current can be excluded.

As is easily visible, the data taken at temperatures down to 0.36 K do not support the occurrence of weak antilocalization, as reported on Si$_{0.3}$Ge$_{0.7}$/Si$_{0.2}$Ge$_{0.8}$/Si$_{0.5}$Ge$_{0.7}$ by Andrievskii et al. [77, 78]. Weak antilocalization is possible in systems with strong spin-orbit interaction. The time-reversed interference paths that lead to weak localization are mixed by spin-orbit interaction to form singlet and triplet channels. While the singlet channel interferes constructively due to the Pauli principle, increasing the probability to return to the point of departure and thereby decreasing conductivity, the triplet channel interferes destructively and therefore increases conductivity. In extreme cases of spin-orbit interaction, the correction to the classical conductivity can be entirely conduction enhancing. In intermediate cases as the one reported in [77, 78], weak antilocalization occurs at
smaller magnetic field scales than the “ordinary” weak localization. Since the spin-orbit interaction in GaAs is similarly strong as the one in Ge, it may be worth noting that in GaAs/Al$_{0.5}$Ga$_{0.5}$As quantum wells [79] there was also no positive magnetoresistance down to a temperature of 350 mK.

Plotting the temperature dependence of the phase breaking time $\tau_\phi$ of the weak localization observed in sample 7404-16 (Fig. 5.7), one observes that $\tau_\phi$ does not diverge with decreasing temperature as would be expected if the dephasing was due to phonons as in (5.27) and (5.28) or due to electron-electron interaction (5.29). Explanations to this fact are not entirely convincing.

The obvious suspicion is that the temperature of the hole gas in the sample does not match the indicated temperature of the cryostat. To clarify this point, the measurement was done using three different currents, 20 nA, 100 nA and 400 nA, corresponding to a 400-fold increase of dissipated heat. Apart from a slight shift of the measured resistance and decreasing noise, there is no noticeable impact of increasing the current. Neither the shape nor the amplitude of the observed weak localization are changed in any way. Fitted curves at 20 nA show decreased characteristic magnetic fields $B_t$ and $B_\phi$, which can be explained by measurement noise. This observation is striking, since a 400-fold increase in energy loss rate to phonons according to (2.1) would imply a drastic increase in hole gas temperature at a lattice temperature of 0.36 K, as discussed in section 2.3.

It was observed that the Shubnikov–de Haas oscillation of some samples, van der Pauw squares to be specific, continue to grow as the indicated temperature is decreased, while SdH oscillations of Hall bar samples cease to grow at about 1 K, independent of the measurement current, consistent with the observation of weak localization saturation. This observation agrees with the notion of heating of the gas, because the large number of carriers in the squares leads to very efficient cooling by phonon emission. It must be stressed again that the effect is independent of the measurement current, excluding the current as a heating source. However, external heating can not be excluded, e.g. by noise coupled into the sample by pickup of the leads.

The fact that some samples show increasing SdH oscillations at least shows that the thermometer of the cryostat cannot be responsible for the observed saturation of weak localization. Further, other, unrelated measurements (i.e. heat capacity of NaCoO$_2$) show that the cryostat thermometer agrees with other independent thermometers.

Intrinsic saturation of the weak localization with decreasing temperature has been observed in thin metal films containing magnetic impurities [80]. In such systems, coherence is destroyed by random spin flips which enables which-path experiments. Magnetic impurities are not necessary, though. Saturation of the weak localization can be observed in a
5.3. ELECTRON-ELECTRON INTERACTION

wealth of systems [81, 82], both 1–dimensional and 2–dimensional. Explanations offered
are gas heating, dephasing by external noise, including particularly microwave radiation
[83]. It has been suggested that zero-point fluctuations causing phase decoherence at low
temperature [84], but this conjecture has been met with a lot of criticism [85, 86].

5.3 Electron-electron interaction

Like weak localization, electron–electron interaction (EEI) is a quantum effect resulting
in a (usually small) correction to the classical resistance. Simply speaking, the electron is
moving in a time dependent electric field created by all electrons in the system. Scattering
by crystal imperfections is the dominant mechanism. On the time scale of secondary
scattering mechanisms, the electron behaves diffusive (rather than ballistic, which is true
for the dominant mechanism).

In the presence of spin degeneracy ( $\epsilon(k, \uparrow) = \epsilon(k, \downarrow)$ ), the conductivity correction due
to EEI is written as [60, 87]

$$\Delta \sigma_{xx} = \frac{e^2}{2\pi^2 \hbar} \left(1 - \frac{3}{4} F^* \right) \ln \frac{k_B T \tau}{\hbar} \quad (5.41)$$

$$\Delta \sigma_{xy} = 0 \quad (5.42)$$

Although the conductivity correction $\Delta \sigma$ does not depend on the magnetic field $B$, the
resistivity correction $\Delta \rho$ does:

$$\Delta \rho_{xx} = -(1 - \mu^2 B^2) \rho_0 \Delta \sigma_{xx} \quad (5.43)$$

$$\Delta \rho_{xy} = -2 R_H B \rho_0 \Delta \sigma_{xx} \quad (5.44)$$

Because it decreases the observed Hall constant $R_H$ according to (5.44), EEI shows itself
by an apparent increase in carrier density as the temperature is decreased.

The interaction parameter $F$ is defined as the angular average of the statically screened
Coulomb interaction $v(q)$, normalized by $v(0)$:

$$F = \frac{\int d\theta v(2k_F \sin \frac{\theta}{2})}{\int d\theta v(0)} \quad (5.45)$$

$$F = \int d\theta \frac{1}{2\pi} \frac{1}{1 + \frac{2k_F}{\kappa} \sin \left(\frac{\theta}{2}\right)} \quad (5.46)$$

where $\kappa$ is the inverse screening length. The appearance of $F$ stems from the interaction
in the Hartree channel, while the exchange channel has the factor 1. The renormalized
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interaction parameter $F^*$ is given by [77][88]

$$F^* = \frac{8}{\pi} \left( 1 + \frac{F^2}{2} \right) \ln \left( 1 + \frac{F^2}{2} \right) - 4. \quad (5.47)$$

The theoretical limits for $F^*$ are 0 (no screening, $\kappa \to 0$, $F \to 0$) and 0.866 (infinite screening, $\kappa \to \infty$, $F \to 1$). If spin degeneracy is assumed, the only role $F^*$ plays is fine-tuning the interaction effect. Literature values for low Ge content quantum wells are $F^* = 0.912$ for Si$_{0.85}$Ge$_{0.15}$ with $p_s = 2.6 \times 10^{11}$ cm$^{-2}$ and $F^* = 0.886$ for Si$_{0.8}$Ge$_{0.2}$ and $p_s = 2.3 \times 10^{11}$ cm$^{-2}$ [89][91].

As virtually any conductivity correction in 2D has $\delta \sigma \propto \ln T$, the different effects are usually detected by investigating the effect of a magnetic field. Due to the Zeeman effect, spin degeneracy is absent, i.e. $\epsilon(k, \uparrow) \neq \epsilon(k, \downarrow)$, and $\Delta \sigma$ becomes field dependent [92][93]:

$$\Delta \sigma_{xx} = \frac{e^2}{2\pi^2 \hbar} (1 - \frac{3}{4} F^*) \ln \frac{k_B T \tau}{\hbar} - \frac{e^2}{2\pi^2 \hbar} \left( \frac{F^*}{2} \right) G_2(h) \quad (5.48)$$

$$G_2(h) = \int_0^\infty d\Omega \frac{d^2}{d\Omega^2} \left[ \Omega N(\Omega) \right] \ln \left| 1 - \frac{h^2}{\Omega^2} \right| \quad (5.49)$$

$$h = \frac{g \mu_B B}{k_B T} \quad (5.50)$$

$$N(\Omega) = (\exp[\frac{\hbar \Omega}{k_B T}] - 1)^{-1} \quad (5.51)$$

$$\Delta \sigma_{xy} = 0 \quad (5.52)$$

$$\Delta \rho_{xx}(B) = \frac{e^2}{2\pi^2 \hbar \sigma_0^2} \left[ (1 - \mu^2 B^2) \left( \frac{F^*}{2} \right) G_2 \left( \frac{g \mu_B B}{k_B T} \right) \right. \right.$$ 
$$\left. - (1 - \mu^2 B^2) \left( 1 - \frac{3}{4} F^* \right) \ln \left( \frac{k_B T \tau}{h} \right) \right] \quad (5.53)$$

with the universal scaling function $G_2$. It behaves as $h^3$ for $h \ll 1$ and as $\ln h$ for $h \gg 1$.

The splitting between spin directions does not have to have a magnetic field as origin, as any destruction of inversion symmetry of the structure will destroy spin degeneracy. Lack of inversion symmetry of the crystal lattice (e.g. in III-V compounds), called built in inversion asymmetry (BIA) or inversion asymmetry due to an asymmetric layer stack (structural inversion asymmetry, SIA) can be the reason. Furthermore, it is not necessary that the eigenfunctions of the zero-field splitting are also eigenfunctions of the Zeeman Hamiltonian. In this case, the bands can never be degenerate at any magnetic field. The term $g \mu_B B$ should then be replaced by a function describing the magnetic field dependence of the band splitting $\Delta \epsilon(B)$. Band structure calculations (chapter 3) suggest that a function $\Delta \epsilon(B)$ of the type $\Delta \epsilon = \epsilon_0 \sqrt{1 + (g \mu_B B/\epsilon_0)^2}$ is an excellent approximation, where $\epsilon_0$ is the band splitting at zero field. This can be understood by observing that the
two heavy hole bands contribute most and equally to the eigenstates of the band structure Hamiltonian. Therefore, the problem can be approximated by a two-level problem with the model Hamiltonian

$$H = \begin{pmatrix} -\epsilon_0/2 & g\mu_B B \\ g\mu_B B & \epsilon_0/2 \end{pmatrix}$$  \hspace{2cm} (5.54)$$

for which the above approximation \(\Delta\epsilon\) is the exact eigenvalue solution.

Electron-electron interaction effects have been found in Si\(_{0.03}\)Ge\(_{0.97}\)/Ge multilayers\(^{94}\) with carrier densities ranging from 2.4 to 2.6\(\times\)10\(^{11}\) cm\(^{-2}\). The aim of our work was to investigate EEI in Si\(_{0.3}\)Ge\(_{0.7}\)/Ge structures with a single channel. We extend the range of the carrier density (1.7 to 5.9 \(\times\) 10\(^{11}\) cm\(^{-2}\)) and the mobility is more than twice the value of the previous study. Apart from the larger strain, our structures are remotely doped from one side, leading to an asymmetric potential that is not expected in multilayers.

In comparing the temperature dependent magnetoresistance (MR) of different samples, one notes that many share an interesting feature. As an example, Fig. 5.8 shows the magnetoresistance of sample 7158-22. At a magnetic field of \(\pm 0.7\) T, the resistance becomes temperature independent. At higher magnetic fields, the resistance increases with increasing temperature, at lower fields, the relation is reversed. Consequently, there is a field \(B_i\) at which the resistance becomes independent of temperature (at least for a reasonably large range of temperatures). In this study, we will concentrate on two of these samples (Table 5.1).

Investigations of the hole density dependence of the crossover require good control over the carrier density. For Schottky type gated samples, this turns out to be limited by the low breakdown voltage that can be achieved using this type of gate on a low band gap semiconductor. The use of silicon dioxide dielectrics permits a much higher gate voltage to be applied. Such samples show a large drift in response to the application of a gate voltage. It is attributed to the charging of traps within the gate oxide.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>(p_s) [cm(^{-2})]</th>
<th>(\mu) [cm(^2)/Vs]</th>
<th>Device No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hall bar</td>
<td>1.66–2.8 (\times) 10(^{11})</td>
<td>20000–43000</td>
<td>7158-22</td>
</tr>
<tr>
<td>square</td>
<td>5.9 (\times) 10(^{11})</td>
<td>75000</td>
<td>6777-2</td>
</tr>
</tbody>
</table>

**Table 5.1:** List of the samples used for this study.
Fig. 5.8: Negative magnetoresistance due to electron-electron interaction, leading to a crossing of the resistivity curves near $B = \pm 0.7 \ T$. In addition, weak localization is observed as a small upturn at lowest $T$ and $B$. Warping of the heavy hole band accounts for the weak positive magnetoresistance best seen in the 14 K data. The over-all appearance is dominated by the electron-electron interaction. Shown is the magnetoresistance of sample 7158-22 at 1.9, 4.0, 8.0, 10.0, 14.0 K (top to bottom).

5.3.1 Drift removal in MOS structures

Sample 7158-22 was fabricated with a 100 nm thick SiO$_2$ gate oxide. Deposited using electron beam evaporation, the oxide contains a high number of defects. When a gate voltage is applied, these defects can trap charge, which has the unwanted effect of reducing gate effectiveness. At low temperature, charging is so slow that the process can take days to finish. Therefore, the amount of charge present in the channel continuously changes during this time. In order to do useful experiments in face of a drifting carrier density, the effects of this drift have to be removed as much as possible. In particular, the location of a common intersection of a set of curves, as in Fig. 5.8, is sensitive to drift.

To quantify the amount of drift experienced by the sample, repeated measurements were performed, as shown in Fig. 5.9. It is evident that the shape of the curves is not much affected by the drift, and the individual curves are symmetric. This shows that the drift during an individual $B$-sweep is negligible.

Analysis of the carrier density and resistance drift over time shows that the relative resistance change $\Delta \rho^{\text{Drift}}/\rho_0$ due to drift is twice as large as the relative hole density change
5.3. ELECTRON-ELECTRON INTERACTION

Fig. 5.9: Drift of the resistance of sample 7158-22 over time is evidenced by $B$ sweeps at 4.0 K (left) and 10.0 K (right). Evidently, the shape of the curves is not affected significantly. The curves are symmetric, which is a clear indication that the drift during a single $B$-sweep is negligible. A slow drift of the carrier density is the reason for the resistance shift, as evidenced by the shift of the minima of the Shubnikov–de Haas oscillations at 4.0 K and observations of the Hall effect (not shown).

$\Delta p_s^{\text{Drift}} / p_s$ and has opposite sign. From this we infer $\rho \propto p_s^{-2}$ which implies $\mu \propto p_s$, where $\mu$ is the mobility. This is in good agreement with the general relation for LEPECVD grown material, as detailed in chapter 4, particularly figure 4.3 (p. 48). Details on the growth mechanism can be found in appendix B.

This analysis allows to scale a set of resistance measurements to a specified carrier density, where the transport parameters can be extracted. Scaled data are shown in Fig. 5.8, 5.10 and 5.11.

5.3.2 Experimental electron-electron interactions

From Eq. 5.53 it follows that for $\mu B = \omega_c \tau_t = 1$, the resistance becomes independent of temperature. Indeed, our samples show this temperature independent field $B_i$ (Fig. 5.8). The overall field and temperature dependence of electron-electron interaction is reproduced.
very well. One notes, however, that the field $B_i$ is larger than one would expect from the measured mobility, which would be $B = \mu^{-1} = 0.23$ T for sample 7158-22 and 0.13 T for sample 6777-2.

As with $B_i$, the amplitude of the effect in $\delta \rho_{xx}$ is larger than predicted by theory. Matching theory to experiment therefore requires scale factors to get amplitude and field dependence right. Interestingly, as will be shown in the following, the curvature of the magnetoresistance follows the expectations from (5.43), and is used to extract the interaction parameter $F^*$. This observation due to the fact that the scalings of $B$ and $\Delta \rho$ offset each other. This may suggest that there is an unidentified mechanism that drives up the zero-field resistance as the temperature falls. When there is a constant curvature caused by electron-electron interaction, the intersection of the magnetoresistance at different temperatures will shift to higher fields.

The higher temperature traces of the magnetoresistance in Fig. 5.8, particularly the 14 K trace, show positive magnetoresistance at fields below 0.25 T. To check whether this effect can be explained by spin-splitting of the bands, we modify (5.53) as following:

$$
\delta \rho_{xx}(B) = C \frac{e^2}{2\pi^2 \hbar \sigma_0^2} \times
\times \left[ (1 - \bar{\mu}^2 B^2) \left( \frac{F^*}{2} \right) G_2 \left( \frac{\alpha \sqrt{\epsilon_0^2 + (3\kappa \mu_B B)^2}}{k_B T} \right) - (1 - \bar{\mu}^2 B^2) \left( 1 - \frac{3}{4} F^* \right) \ln \left( \frac{T}{T_0} \right) \right]
$$

(5.55)

where $\bar{\mu}$ is the modified mobility, $C$ is a scale factor, $\epsilon_0$ represents the zero field band splitting, $3\kappa \mu_B B$ represents the Zeeman energy of a heavy hole in Ge, where $\kappa$ is the corresponding Luttinger parameter [95] and $F^*$ is an interaction parameter.

The resistance scale factor $C$ is expected to be of order unity, as is the scaling factor of the mobility. The overall form, especially at the low end of the temperature scale, can be well reproduced by Eq. (5.55) even when the Zeeman term is omitted. Fitting the distinct positive magnetoresistance that is observable from Figure 5.8 at temperatures above 8 K however requires the use of a large $\alpha$. This ad hoc parameter is required to take values around 10–20, depending on the sample and the value of $F^*$, such a scaling would have to be identified with an unphysical scaling of the temperature by a factor of 10–20. The observed positive magnetoresistance therefore is not meaningfully ascribed to electron-electron interaction.

Instead of resorting to an inflated Zeeman term, the positive magnetoresistance above 8 K may be ascribed to the semiclassical band structure effect [71], described in section 5.1.
Fig. 5.10: Magnetoresistance of sample 7158-22 at 1.9, 4.0, 6.0, 8.0, 10.0 and 14.0 K (arrows) as function of $B^2$ (solid lines). The dashed lines are fits to the field range 0.5–0.7 T. The weak upturn of the data at smallest $B$ is due to weak localization. The remaining background is essentially temperature independent. It is suspected to be a semiclassical band structure effect caused by the warping of the heavy hole band in Germanium. The carrier density was $2.75 \times 10^{11}$ cm$^{-2}$.

Since in the temperature range studied using sample 7158-22 we have $T \ll T_F = \epsilon_F/k \approx 70$ K, this semiclassical effect should lead to a temperature independent magnetoresistance. This is expected to be even more pronounced for the case of sample 6777-2, shown in Figure 5.4. The band warping increases with energy, and at a carrier density of $p_s = 5.9 \times 10^{11}$ cm$^{-2}$ it dominates the field dependence of the magnetoresistance. The temperature dependence of the magnetoresistance is ascribed to electron-electron interaction.

To separate the band structure effect from the electron-electron interaction effect, we make use of the different field scales at which the effects take place. While the first leads to positive magnetoresistance for $|B| < \mu^{-1}/2$, the second prevails at much higher fields.
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Fig. 5.11: Magnitude of the electron-electron interaction effect on the resistivity for six hole densities, measured by the slopes of the dashed lines in Fig. 5.10. A log($T$) dependence is expected for electron-electron interaction and the characteristic temperature increases with increasing hole density.

By fitting a parabola of the form $\rho_{xx}(B) = \rho_{xx}^{(0)} + \rho_{xx}^{(1)}B + \rho_{xx}^{(2)}B^2$ in the field range $0.5 < |B| < 0.7$ we stay well beyond the field for which the band structure effect modifies the resistance, yet we do not enter the regime of Shubnikov–de Haas oscillations. The result is shown in Figure 5.10 (sample 7158-22 with a hole density of $2.77 \times 10^{11}$ cm$^{-2}$). There, Fig. 5.8 is replotted with $B^2$ as $x$-axis, so that parabolas appear as straight lines in the plot. As can be seen, the fits do capture the basic effect of electron-electron interaction very well.

At very small fields, the measured curves turn up, forming the familiar weak localization peak. Taking this weak localization into account, quantitative analysis shows that the difference between the parabolic fits and the measured curves is essentially temperature independent, as expected for the band structure effect.

To quantify the electron-electron interaction effects, we plot the second order coefficient $\rho_{xx}^{(2)}$ of the mentioned fit against the temperature (Figure 5.11) for sample 7158-22, and
Fig. 5.12: The interaction parameter $F^*$ in Ge/Si$_{0.3}$Ge$_{0.7}$ (▲) increases with carrier density $p_s$. The results are consistent with a value of 0.912 for Si$_{0.85}$Ge$_{0.15}$ (○) where $p_s = 2.6 \times 10^{11}$ cm$^{-2}$ obtained by Senz et al. [90] and 0.886 for Si$_{0.8}$Ge$_{0.2}$ (▼) and $p_s = 2.3 \times 10^{11}$ cm$^{-2}$ found by Emeleus et al. [89].

A perfect log $T$ behavior is found for six different values of the carrier density. According to (5.41) in combination with (5.43), the temperature $T_0$ at which $\rho^{(2)}_{xx}$ becomes zero is associated with a characteristic time scale $\tau = \hbar/k_B T_0$. We find a characteristic time scale $\tau = 5 \times 10^{-13}$ s from the temperature $T_0 = 15$ K at with $\rho^{(2)}_{xx} = 0$ at a hole density of $2.77 \times 10^{11}$ cm$^{-2}$, as shown in Fig. 5.11. As the carrier density is reduced from this value, $T_0$ shifts to lower temperatures while the magnitude of the effect and $\tau$ both increase. The time scale $\tau$ is significantly shorter than the momentum relaxation time $\tau_{tr} = 2.1 \times 10^{-12}$ s derived from the carrier mobility, and is close to the quantum scattering time $\tau_q = 0.33$ ps, the lifetime of a quantum mechanical state.

Combining (5.41) and (5.43), the interaction constant $F^*$ can be found from the $B^2$–term of the magnetoresistance in Fig. 5.11. The interaction parameter increases with increasing carrier density, as shown in Fig. 5.12. The size and density dependence of $F^*$ indicates efficient screening at higher carrier densities that gradually becomes weaker as the carrier density is reduced.

The characteristic temperature $T_0$ is the temperature at which the resistance contribution of the interaction effects is independent of $B$. In absence of other magnetoresistive effects, the equation $\rho(B = 0) = \rho(B = B_i)$ holds at $T = T_0$, which can be used to find $T_0$. 


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**Fig. 5.13:** The electron-electron interaction is expected to increase $R_H$ as temperature decreases. The opposite behavior is observed, and as the two temperature sweeps show, a drift of the carrier density over time can be ruled out.

However, this method requires taking care of the band structure induced magnetoresistance and is also susceptible to drift effects. Therefore, $T_0$ data points found in this way show considerably larger spread.

In principle, since $\delta \sigma_{xy} = 0$, one would expect that the observed quantum correction in the transversal resistance is related to the longitudinal quantum correction by

$$\delta R_H = 2R_H \frac{\delta \rho}{\rho_0} \quad (5.56)$$

However, this is not observed. The Hall effect of the sample 7158-22 increases with temperature as shown in Fig. 5.13, while $\delta \rho$ decreases with increasing temperature. The difference in carrier density corresponding to this change of the Hall constant is $4.3 \times 10^9 \text{ cm}^{-2}$, or 2.5%.
5.4 Conclusions

We have found an interesting instance of negative magnetoresistance in strained Ge channels. The overall temperature and field dependence of the effect can be well described by electron-electron interaction. In particular, we observe a temperature independence of the longitudinal resistance at a particular field. For several values of the carrier density we were able to extract the interaction parameter $F^*$ from the curvature of the magnetoresistance. The magnetic field needed to achieve temperature independence of the resistance is more than three times larger than expected from theory applying the basic theoretical prediction to an ideal 2D gas. The resistance range difference between the temperature independent value and the $B = 0$ value exceeds the theoretical value by the same factor. The curvature, however, follows the theoretical expectations and the values of the interaction parameter we find from it are very consistent with the values observed in SiGe heterostructures with low Ge content.

The electron-electron interaction induced magnetoresistance is superposed on a temperature independent positive magnetoresistance which presumably originates from the warping of the heavy hole band in Germanium. The combined effects provide an excellent description of the magnetoresistance of strained Ge channels with hole densities between 1.7 to $5.9 \times 10^{11}$ cm$^{-2}$. However, it should be mentioned that at least for high carrier density a second explanation for the observed low field magnetoresistance exists, namely the occupation of additional subbands.

The weak localization has been investigated. The effect shows saturation at temperatures of less than 1 K. Whether this effect is intrinsic or caused by external heating could not be clarified. Heating by the measurement current itself can be excluded, however. Future work should certainly attempt to shed light on the interesting question whether there is intrinsic saturation of weak localization in these samples.
Conclusions and Outlook

In this work we present fundamental properties of strained Ge films in SiGe substrates. Effective mass, scattering mechanisms and the mobility as well as quantum corrections to electrical transport in small magnetic fields and band structure induced magnetoresistance have been investigated.

The principal scattering mechanisms in electric transport have been clarified by mobility measurements at 2.0 K. The samples used in the study have the highest mobility reported so far for this material system with a peak mobility of 120'000 cm$^2$/Vs at a carrier density of $8.5 \times 10^{11}$ cm$^{-2}$. Charged states at the channel–cladding interfaces have been identified as the main scattering mechanism. This mechanism has also been reported for Si$_{0.3}$Ge$_{0.7}$/Si samples, grown by MBE. The occurrence of the same scattering mechanism in material grown by fundamentally different growth processes suggests that the limits of the mobility are related to intrinsic properties of the material rather than process related. The atomic nature of the interface has not yet been clarified. As increased mobility has been reported for higher strained layers, optimizing the mobility by strain adjustment is a promising subject.

The dependence of the effective mass on the sheet carrier density, i.e. energy, has been investigated in detail. Calculations have been performed that agree very well with experiment. The apparent discrepancy between the mass measured in a magnetic field and the mass calculated from the zero-field band dispersion has been shown to be a direct consequence of band non-parabolicity. Reproduction of the measurement with a calculation yielded excellent agreement of experiment and calculation. When the mobility is phonon limited, the limit will be lower than suggested by measured mass because the zero-field mass is larger, particularly at high carrier density, which is technically most interesting.

Quantum corrections to electrical transport are noticeable only at low carrier densities, where conductivity corrections are larger compared to the classical conductivity than at higher carrier density. Electron-electron interactions lead to a temperature dependent zero-field resistance and a parabolic negative magnetoresistance. Interestingly, the relevant
scattering time associated with the temperature dependence of the effect seems to be almost independent of the carrier concentration. Future work on this matter could address the temperature dependence of the weak localization at $T < 1 \text{ K}$, particularly the question whether the saturation effects are intrinsic to the samples or due to imperfections of the measurement setup.

As this work and the work of others have shown, strained germanium films have great electronic properties that make it an excellent material for future electronic applications. The future problems to solve on the way to introduction in commercial devices seem to lie in the area of using the strained film in on-insulator technology and in the fabrication of a (high-k) gate dielectric.

Fabricated Ge/SiGe quantum wells have reached a level of quality that makes it possible to use them for quantum transport experiments like quantum point contacts, single electron transistors and others.
Appendix A

Band parameters of Si, Ge and SiGe

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
<th>Si$<em>x$Ge$</em>{1-x}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ [Å]</td>
<td>5.419770(19)</td>
<td>5.646133(10)</td>
<td>see eq. A.1</td>
</tr>
<tr>
<td>band gap $E_g$ [eV]</td>
<td>1.12</td>
<td>0.66</td>
<td></td>
</tr>
<tr>
<td>dielectric constant $\epsilon$</td>
<td>11.8</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>$E_0$ [eV]</td>
<td>4.229 (Γ$<em>{25v'}$–Γ$</em>{2'c}$)</td>
<td>0.898(1) (Γ$<em>{8v}$–Γ$</em>{7c}$)</td>
<td></td>
</tr>
<tr>
<td>$E'_0$ [eV]</td>
<td>3.40 (Γ$<em>{25v'}$–Γ$</em>{15c}$)</td>
<td>3.206 (Γ$<em>{8v}$–Γ$</em>{8c}$)</td>
<td></td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>4.26</td>
<td>13.38(2)</td>
<td></td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>0.38</td>
<td>4.24(3)</td>
<td></td>
</tr>
<tr>
<td>$\gamma_3$</td>
<td>1.56</td>
<td>5.69 (2)</td>
<td></td>
</tr>
<tr>
<td>$\kappa$</td>
<td>-0.26</td>
<td>3.41(3)</td>
<td></td>
</tr>
<tr>
<td>$q$</td>
<td>0.01</td>
<td>0.06(1)</td>
<td></td>
</tr>
<tr>
<td>$E_p$ [eV]</td>
<td>21.6</td>
<td>26.3</td>
<td></td>
</tr>
<tr>
<td>$a = D_d$ [eV]</td>
<td>12.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$b = -\frac{2}{3} D_u$ [eV]</td>
<td>-2.10(10)</td>
<td>-2.4(4)</td>
<td></td>
</tr>
<tr>
<td>$d = -\frac{2}{\sqrt{3}} D_{u'}$ [eV]</td>
<td>-4.84(10)</td>
<td>-5.0</td>
<td></td>
</tr>
<tr>
<td>$c_{11}$ [GPa]</td>
<td>165</td>
<td>129</td>
<td></td>
</tr>
<tr>
<td>$c_{12}$ [GPa]</td>
<td>63</td>
<td>48</td>
<td></td>
</tr>
<tr>
<td>$c_{44}$ [GPa]</td>
<td>79</td>
<td>67</td>
<td></td>
</tr>
<tr>
<td>$\nu$ (Poisson ratio)</td>
<td>0.28</td>
<td>0.27</td>
<td></td>
</tr>
</tbody>
</table>

*a* hydrostatic compression  
*b* uniaxial compression, values vary a lot  
*c* uniaxial shear

**Table A.1: Properties of Si and Ge**
\[ a(x) = a(0) + 0.20036x(1-x) + [a(1) - a(0)]x^2 \]  
\hspace{1cm} (A.1)

### A.1 Interpolation of band parameters

Nonlinear interpolation of the band parameters follows the work of Lawaetz [96], who used results of the \( k \cdot p \) method to predict the valence band parameters of various group IV and III-V semiconductors.


<table>
<thead>
<tr>
<th></th>
<th>Si ((x = 0))</th>
<th>Ge ((x = 1))</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-s gap ( E_0 ) [eV]</td>
<td>4.07</td>
<td>0.89</td>
</tr>
<tr>
<td>p-p gap ( E'_0 ) [eV]</td>
<td>3.40</td>
<td>3.16</td>
</tr>
<tr>
<td>( X - \Gamma' ) matrix element ( E_P ) [eV]</td>
<td>21.6</td>
<td>26.3</td>
</tr>
<tr>
<td>( X - \Gamma_{15} ) matrix element ( E'_P ) [eV]</td>
<td>14.4</td>
<td>17.5</td>
</tr>
<tr>
<td>( \bar{\gamma}_1 )</td>
<td>-0.3323</td>
<td>-0.1623</td>
</tr>
<tr>
<td>( \bar{\gamma}_2 )</td>
<td>0.20133</td>
<td>0.2378</td>
</tr>
<tr>
<td>( \bar{\gamma}_2 )</td>
<td>-0.0303</td>
<td>-0.1587</td>
</tr>
<tr>
<td>( \bar{\gamma}_2 )</td>
<td>-0.4387</td>
<td>-0.59217</td>
</tr>
<tr>
<td>( D )</td>
<td>1</td>
<td>1.261</td>
</tr>
</tbody>
</table>

Interpolation of the valence band parameters of \( \text{Si}_{1-x}\text{Ge}_x \):

\[ D(x) = D(1)x + D(0)(1-x) \]  
\hspace{1cm} (A.2)

\[ E_0(x) = E_0(1)x + E_0(0)(1-x) \]  
\hspace{1cm} (A.3)

\[ E'_0(x) = E_0(0) \left( \frac{a(x)}{a(0)} \right)^{-1.92} \]  
\hspace{1cm} (A.4)

\[ E_P(x) = E_P(0)\{1 + 1.23[D(x) - 1]\} \left( \frac{a(x)}{a(0)} \right)^2 \]  
\hspace{1cm} (A.5)

\[ E'_P(x) = E'_P(0)\{1 + 1.23[D(x) - 1]\} \left( \frac{a(x)}{a(0)} \right)^2 \]  
\hspace{1cm} (A.6)

\[ \bar{\gamma}_1 = \bar{\gamma}_1(1)x + \bar{\gamma}_1(0)(1-x) \]  
\hspace{1cm} (A.7)

\[ \bar{\gamma}_2 = \bar{\gamma}_2(1)x + \bar{\gamma}_2(0)(1-x) \]  
\hspace{1cm} (A.8)

\[ \bar{\gamma}_3 = \bar{\gamma}_3(1)x + \bar{\gamma}_3(0)(1-x) \]  
\hspace{1cm} (A.9)

\[ \bar{\kappa} = \bar{\kappa}(1)x + \bar{\kappa}(0)(1-x) \]  
\hspace{1cm} (A.10)
A.1. INTERPOLATION OF BAND PARAMETERS

\begin{align*}
\gamma_1 &= \frac{1}{3} \frac{E_P}{E_0} + \frac{1}{3} \frac{E'_P}{E'_0} + \bar{\gamma}_1 \quad (A.11) \\
\gamma_2 &= \frac{1}{6} \frac{E_P}{E_0} - \frac{1}{6} \frac{E'_P}{E'_0} + \bar{\gamma}_2 \quad (A.12) \\
\gamma_3 &= \frac{1}{6} \frac{E_P}{E_0} + \frac{1}{6} \frac{E'_P}{E'_0} + \bar{\gamma}_3 \quad (A.13) \\
\kappa &= \frac{1}{6} \frac{E_P}{E_0} - \frac{1}{6} \frac{E'_P}{E'_0} + \bar{\kappa} \quad (A.14)
\end{align*}

\textbf{Fig. A.1:} Valence band parameters of Si}_{1-x}Ge$_x$ alloys.
Appendix B

LEPECVD

The Low Energy Plasma Enhanced Chemical Vapour Deposition (LEPECVD) growth system used to deposit the complete layer stack of the SiGe/Ge quantum wells consists of a wafer stage, a process gas inlet, a plasma source, a vacuum vessel and a pump assembly [12, 97–102]. During deposition, the plasma source generates a high density, low voltage plasma that is directed toward the wafer by a magnetic field. The plasma intensity can be varied both by changing the plasma discharge current as well as by changing the coil current that controls the magnetic confinement of the plasma. The plasma is produced in an argon flow fed into the plasma source. Due to the action of the pump system, the plasma flows into the deposition chamber.

The process gas is fed into the deposition chamber through a circular inlet in the vicinity of the wafer. Gaseous compounds of the deposition materials are used as precursor gas. The system uses germane (GeH₄), silane (SiH₄) and diluted diborane (100 ppm B₂H₆ in Ar). The plasma excites the precursor molecules and produces reactive radicals. When they impinge on the wafer surface, the materials are incorporated into the crystal lattice, while the hydrogen is stripped and forms a layer on the wafer surface. Energy transfer from plasma components hitting the wafer surface are assumed to help dissociation of the hydrogen from the surface. All precursor gas is decomposed in the plasma, so that only hydrogen and argon can leave the deposition chamber through the pumps.

In conventional Chemical Vapour Deposition (CVD), the precursor gas is adsorbed to the hot wafer surface, where the molecules are decomposed. The decomposition is thermally activated, which makes the maximum growth rate exponentially dependent on the wafer temperature. Due to the different energy required for decomposition of different precursor compounds, the solid deposited by conventional CVD has a different composition than the gas mixture used. Catalytic influence of one species on the deposition rate of another species is also possible. The composition of the solid is also temperature dependent, since
at high temperatures the solid composition tends toward the gas composition, especially if the deposition rate is low (the reaction is limited by the availability of precursors). The desorption of hydrogen from the surface of the wafer is another thermally activated step. Whether the decomposition or hydrogen desorption limit the deposition rate depends on the species that are being deposited.

The advantage of the plasma assisted system over a CVD system is based on the production of reactive species and hydrogen removal. Reactive species do not have to be decomposed on the wafer surface by thermal processes. Hydrogen removal is assumed to be aided by ion bombardment from the plasma, removing this process as a rate limiting step.

Decoupling the growth rate from the temperature is the greatest virtue of LEPECVD. One has to keep in mind that SiGe heterostructures require temperature control to achieve the desired quality. The deposition of strain relaxed buffers requires efficient strain relaxation, i.e. long dislocation loops or a low density of threading arms penetrating the surface. Strained layer growth requires suppression of strain relaxation, since the strained layers frequently are thicker than the equilibrium thickness. These requirements force conventional CVD to operate in a temperature range that is not suitable for fast, efficient deposition. LEPECVD, on the other hand, achieves high growth rates at optimal deposition conditions and high gas utilization.
Appendix C

Sample Processing

For the fabrication of Hall bars, we used conventional photolithography. The photoresist was Clariant AZ 9260 thick film positive h/i-line resist. At the spinning speed of 4000 rpm, the final film thickness is 6 µm. This relatively thick film was chosen to limit possible effects of HF diffusion during the mesa etch. The sample damage related to HF will be discussed in the course of this appendix. After the spinning, the samples were stored for 15 minutes inside their boxes to give the film time to relax stress resulting from the spinning. The softbake was done at 100 °C for 240 s. During the next 30 minutes the samples were allowed to rest, so that the film could absorb water. Water is needed for the photochemical reaction during exposure, and lack of water degrades the contrast available, leading to smeared features. The samples were then exposed to UV light from a Karl Suss mask aligner for 120 s. The relatively long exposure time is explained by the low content of photosensitive compounds in thick film resist. This is required because the photosensitive compounds absorb UV light. Therefore, to assure sufficient and even exposure throughout the film, the content of such compounds has to be limited. The developer was AZ 400K, diluted with water at a ratio of 1:4. The sample was immersed in the developer inside a petri dish for 4 minutes. Fresh developing solution was used for every sample when several samples were processed simultaneously. Removal of the photoresist after processing or for liftoff was performed using acetone or AZ Remover. For metal liftoff, ultrasound was used to speed up the metal removal.

The etch bath for the mesa etch consists of 7 ml HF, 51 ml HNO₃ and 40 ml H₂O. At the bath temperature of 35 °C , stabilized by immersion in a large water bath, the etch rate is 25 nm/s into Si₀.₃Ge₀.₇. Depending on the etch depth required, the etch was done for 10 s or 20 s during which the sample was moved in the solution. A general feature of this type of etch is that the etch rate increases with silicon content. Therefore, the reaction on the unprotected back of the wafer is violent, producing a large amount of gas and generally
leaving brown stains on the surface.

After mesa fabrication, ohmic contacts to the sample were made by depositing 200 nm Al and 100 nm Ag by a lift off process. The definition of the windows in the resist was followed by a short HF dip to remove the oxide from the sample surface, hoping that the reoxidation process would be slow. The metal was then evaporated onto the sample using an e-beam evaporator. After liftoff, the samples were annealed at 400 °C for 60 minutes using the heater stage of the LEPECVD system. The originally very flat, shiny metal surface becomes rough and matte during this process. There was no optimization of the annealing process since there was no obvious gain from a shorter anneal.

Gates, if added, were made from 100 nm Ti covered by 200 nm Ag, patterned by liftoff. Given the high number of samples produced and the long storage times that were a consequence thereof, silver as cover layer was not the optimal choice. Its tendency to oxidize made wire bonding at a later time very difficult, if not impossible. The gates then have to be contacted using silver epoxy or silver paint, a method that requires a steady hand and is prone to producing electrical shorts. Gold would be a better choice for the future.

**Fig. C.1:** Wet etching of the mesa using HF/HNO$_3$/H$_2$O and oxide removal before gate deposition both lead to staining (bright stripes) of the mesa top around the edges of the mask, probably caused by reaction of HF with the oxidized top layers. The contact metallisation (left) shows great roughening during the contact annealing process, while the gate (right) is not annealed and remains very flat. Its surface texture shows the oxidation of the silver cover layer.
The pattern transfer with the mesa etch is good as far as the shape of the Hall bar is concerned. The position of the mesa edge is precisely where defined with the resist. The aspect ratio of the mesa side walls is approximately 1:2, which is relatively flat but tolerable. Around the top border of the mesa there is an area of about 4 $\mu$m width which shows different contrast in SEM images than the rest of the mesa surface. This contrast change can also be observed in the area of the mesa that was covered by resist, but within about 4 $\mu$m of the window that was subjected to an HF dip during preparation of the contacts. Since HF is the only aggressive ingredient shared by both solutions, it is likely that HF has diffused along the interface of resist and sample during the etching. AFM measurements of the transition across the contrast change show that there is a step of about 7 nm height associated with it. The step can also be observed through differential interference contrast optical microscopy. However, it is difficult to notice at all if one is not specifically looking for it.

The step is much lower than the thickness of the upper cladding of the quantum well. The problem associated with it is that the changed surface structure is likely to change the type of surface states at the sample surface. This in turn changes the band alignment at the sample surface. The result is a change of the carrier density underneath the affected surface. This also means that the sample properties are no longer spatially uniform. The surface of the thin voltage probes to the sides of the Hall bar seem to be completely changed. As these contacts fail when the gate is biased such that the carrier density is reduced, it is likely that the carrier density around the border of the sample has been reduced.
## Table C.1: Sample Preparation

<table>
<thead>
<tr>
<th>Step</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Adhesion promoter</strong></td>
<td>TI Prime</td>
</tr>
<tr>
<td><strong>Photoresist</strong></td>
<td>AZ 9260</td>
</tr>
<tr>
<td><strong>Developer</strong></td>
<td>AZ 400K (MIC)</td>
</tr>
<tr>
<td><strong>Remover</strong></td>
<td>AZ 100</td>
</tr>
<tr>
<td><strong>Mesa etch</strong></td>
<td>adhesion promoter 4000 rpm, 5000 rpm/s, 40s</td>
</tr>
<tr>
<td></td>
<td>100 °C , 120 s</td>
</tr>
<tr>
<td></td>
<td>resist spinning 4000 rpm, 5000 rpm/s, 40 s</td>
</tr>
<tr>
<td></td>
<td>9000 rpm, 5000 rpm/s, 5 s (suppresses edge-beads)</td>
</tr>
<tr>
<td></td>
<td>soft bake 100 °C , 240 s</td>
</tr>
<tr>
<td></td>
<td>exposure 120 s</td>
</tr>
<tr>
<td></td>
<td>developer 22-25 °C , 240 s (1.5 µm /min)</td>
</tr>
<tr>
<td></td>
<td>hard bake 105-110 degC, 120 s</td>
</tr>
<tr>
<td></td>
<td>etch bath 7 ml HF, 51 ml HNO₃ and 40 ml H₂O</td>
</tr>
<tr>
<td></td>
<td>35 °C , 10 s or 20 s (25 nm/s)</td>
</tr>
<tr>
<td><strong>contact pads</strong></td>
<td>photolithography like mesa, no hard bake</td>
</tr>
<tr>
<td></td>
<td>metal stack 200 nm Al, 100 nm Ag (e-beam evaporation)</td>
</tr>
<tr>
<td></td>
<td>contact anneal 400 °C , 1 h</td>
</tr>
<tr>
<td><strong>gates</strong></td>
<td>photolithography like contacts</td>
</tr>
<tr>
<td></td>
<td>metal stack 100 nm Ti, 200 nm Ag (e-beam evaporation)</td>
</tr>
</tbody>
</table>
List of Publications

1. B. Rößner, H. von Känel, D. Chrastina, G. Isella, and B. Batlogg, Limitations of effective mass extraction from Shubnikov–de Haas oscillations. submitted for publication


List of Presentations

1. Hole band nonparabolicity and effective mass measurement in p-SiGe/Ge heterostructures, European Materials Research Society Spring Meeting 2006, Nice, France, June 1, 2006 (talk)

2. Low-temperature transport in high quality strained Ge channels in SiGe, Annual APS March Meeting 2006, Baltimore, USA, March 16, 2006 (talk)


4. Electron interaction effects in strained p-SiGe/Ge heterostructures, First International Workshop on New Group IV Semiconductor Nanoelectronics, Sendai, Japan, May 27, 2005 (talk+poster)

5. 2-D Hole Gas with Two-Subband Occupation in a Strained Ge Channel: Scattering Mechanisms, Fourth International Conference on Silicon Epitaxy and Heterostructures, Awaji Island, Hyogo, Japan, May 23, 2005 (poster)

6. Quantum hall effect studies in high mobility p-Ge/SiGe quantum wells, Annual APS March Meeting 2004, Montreal, Canada, March 16, 2004 (talk)

7. Scattering mechanisms in very high mobility p-Ge/SiGe quantum wells, Annual APS March Meeting 2004, Montreal, Canada, March 16, 2004 (talk)

8. High Mobility Hole Gases in compressively strained Ge quantum wells, 12th Euro-MBE Workshop, Bad Hofgastein, Austria, February 17, 2003 (poster)

References


REFERENCES


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