Active manipulation of the g-tensor in semiconductor nanostructures

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Active manipulation of the g-tensor in semiconductor nanostructures

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de rector magnificus prof.dr.ir. F.P.T. Baaijens, voor een commissie aangewezen door het College voor Promoties, in het openbaar te verdedigen op donderdag 17 december 2020 om 16:00 uur

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Cover art: strain profile on the cross-sectional plane of a nanowire quantum dot calculated in Chapter 6 (Fig. 6.2). The background is a pattern of alternating electron and hole wavefunctions in a self-assembled quantum dot calculated in Chapter 4 (Fig. 4.7a and 4.7c). The title is accompanied by a scanning electron microscopy image of the nanowire on which the majority of the measurements presented in Chapter 7 has been performed (Fig. 7.2c).

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# Table of contents

1 Introduction 1
   1.1 Outline of this thesis ................................. 5

2 Theory 7
   2.1 Introduction ........................................... 8
   2.2 Zinc Blende & Wurtzite crystal structures .............. 9
   2.3 Elasticity tensor and response to stress ............... 11
   2.4 Band structure ......................................... 15
   2.5 $k\cdot p$-theory ....................................... 18
   2.6 Spin Hamiltonian ........................................ 23
   2.7 Diamagnetic shift ...................................... 27

3 Experimental techniques 31
   3.1 Introduction ........................................... 32
   3.2 Characterization setup .................................. 32
   3.3 Magneto-luminescence setup ............................. 33

4 Numerical calculations of a strained self-assembled quantum dot 37
   4.1 Introduction ........................................... 38
   4.2 Details of the numerical model ......................... 38
   4.3 Strain calculations ..................................... 39
   4.4 Electronic calculations ................................ 42
   4.5 Magnetic field .......................................... 43
   4.6 Strain-dependence of the g-tensors ..................... 45
   4.7 Diamagnetic shift ...................................... 52
   4.8 Conclusions ............................................ 55

5 Active tuning of the g-tensor in InGaAs/GaAs quantum dots 57
   5.1 Introduction ........................................... 58
   5.2 Device fabrication ...................................... 58
   5.3 Device characterization ................................ 60
   5.4 Magneto-optical measurements .......................... 61
   5.5 Strain-dependence of the g-tensors ..................... 65
   5.6 Diamagnetic shift ...................................... 68
   5.7 Conclusions ............................................ 70
6 Strain and g-tensors in an InAsP nanowire quantum dot  
6.1 Introduction ................................................. 74  
6.2 Wurtzite parameters for InAs and InP ......................... 76  
6.3 Strain calculations ........................................... 80  
6.4 Strain-dependence of the band edges ............................. 84  
6.5 Quantization energy .......................................... 86  
6.6 Electron g-factor in WZ materials ............................... 88  
6.7 Strain-dependence of the electron g-factor ....................... 91  
6.8 Valence band g-factors ....................................... 92  
6.9 Conclusions .................................................. 95  

7 Magneto-optical characterization of a strained nanowire quantum dot  
7.1 Introduction .................................................. 98  
7.2 Sample fabrication ............................................ 98  
7.3 Sample characterization ...................................... 101  
7.4 Magneto-optical measurements ................................ 106  
7.5 Resolving the full g-tensor ................................... 118  
7.6 Conclusions .................................................. 123  

Summary ......................................................... 125  

Acknowledgements ................................................. 129  

Curriculum Vitae .................................................. 132  

List of publications ............................................... 133  

References ....................................................... 134
Chapter 1

Introduction
Chapter 1. Introduction

In the second half of the twentieth century the development of electronics has driven us towards an information society. To meet the ever-increasing demand of more and faster data processing, new ideas are being proposed and new techniques are being developed continuously. Quantum dots (QDs) [1] are semiconductor nanostructures and have often been suggested as fundamental building blocks for future quantum technologies, as they can be utilized as sources of single photons or hosts of quantum bits [2]. The single electrons and holes confined in a QD carry besides a charge also a spin, which can be used as a degree of freedom to store and process information. The possibility to use the spin of a charge carrier as a means to store and process information has given rise to the field of spintronics [3]. The ability to control spins is at the center of this field.

Coupling spin to an externally applied magnetic field leads to an energy difference between the two spin states, which was first discovered by Pieter Zeeman in 1897 [4] and therefore referred to as the Zeeman splitting. Interestingly the discovery of Zeeman preceded the discovery of spin by nearly thirty years. It was Wolfgang Pauli who in 1925 reported a two-valuedness of the electron [5], which later that year was described by Uhlenbeck and Goudsmit as a clockwise or counterclockwise rotation of the electron which they called spin [6]. It was later established by Dirac that an electron does not physically rotate, but that spin rather is an intrinsic angular momentum [7] which can interact with magnetic fields. This interaction can be exploited to gain control over the spin of an electron in a QD by manipulating an externally applied magnetic field [8]. A disadvantage of this approach lies within the difficulty of locally generating magnetic fields, which makes it unsuitable for the manipulation of the spins on a single QD level. Another method of achieving the same result is not to manipulate the magnetic field itself, but rather the interaction of the electron with the magnetic field. This interaction is characterized by the g-tensor. A new method to gain control over this g-tensor is the main topic of investigation in this thesis. The g-tensor contains all information about the magnetic moment of a charge carrier which can have different contributions. The different components of the g-tensor are referred to as g-factors. In many instances the g-tensor is isotropic and can be reduced to a single g-factor. An electron in free space for example only carries its intrinsic magnetic moment, spin, which yields a single g-factor with a value of 2. In fact, quantum field theory introduces a small correction which is omitted here, and the free electron g-factor actually has a value of roughly 2.0023 and is one of the most accurately known constants in physics. An electron bound to an atom can, besides its spin, also carry an orbital angular momentum, leading to the well-known Landé g-factor. When this atom is located in a crystal lattice,
such as a semiconductor, the Bloch theorem states that the wavefunction of an
electron can be expressed as the product of a plane wave and a function with the
periodicity of the crystal lattice. This leads to an extended state which then has
a significant contribution to the electron g-factor. In a semiconductor crystal the
bottom conduction band consists out of $s$-like states which do not contribute to
the orbital part of the g-factor. The g-factor of a conduction band state then re-
duces to the free electron value of 2 when coupling to other bands is neglected. In
a true semiconductor crystal, an electron in the conduction band is never a pure
conduction band state due to the finite band gap and the mixing with the valence
band states becomes relevant. It is this contribution from the valence band states
which causes the electron g-factor in III-V semiconductors to deviate strongly from
the free electron g-factor with a value of 2. This was first established using second
order perturbation theory for ZB materials already in the late fifties by Roth et
al. [9], resulting in a compact formula given by

$$g_e = 2 - \frac{2E_P\Delta}{3E_g(E_g + \Delta)}, \quad (1.1)$$

where $E_g$ is the band gap, $\Delta$ the spin-orbit coupling and $E_P$ the Kane energy
related to $s$- and $p$-like orbitals. This is nowadays known as the Roth formula and is
able to accurately reproduce experimentally known values for the electron g-
factor in common III-V semiconductors such as InAs, GaAs and InP, the materials
that are mainly used in the work presented in this thesis. Experimental values for
the g-factors for direct gap III-V semiconductors are 1.26 for InP [10], -0.44 for
GaAs [11, 12], -7.8 for GaSb [13], -14.7 for InAs [14] and -51.3 for InSb [15]. The
extreme value for InSb, which has a narrow gap combined with a large spin-orbit
interaction, is no surprise since the Roth formula immediately illustrates the crucial
role of the spin-orbit interaction; without spin-orbit interaction the contributions
from the different valence bands to the electron g-factor cancel each other out,
resulting in the free electron g-factor of 2.

Even though the Roth formula works well for bulk materials, it fails to describe
the electron g-factor in nanostructures such as quantum dots. A nanostructure
breaks the periodicity of the crystal and therefore affects the g-factor. Size quan-
tization increases the separation between states in the conduction band and states
in the valence bands, leading to an effective gap which is always larger than the
band gap of the bulk material, therefore bringing the electron g-factor close to the
free electron g-factor of 2. However, this effect alone is not sufficient to explain the
often-observed anisotropy in the g-tensor in semiconductor nanostructures [16, 17].
To understand this one has to consider the spin-correlated currents, created by the
spin-orbit interaction, which are linked to the orbital contribution to the electron
Chapter 1. Introduction

g-factor [18, 19]. The spatial confinement introduced by the nanostructure limits the extension of these spin-correlated currents and therewith the orbital contribution to the electron g-factor, a concept known as orbital momentum quenching [20, 21]. The asymmetry of the confining potential of the nanostructure then leads to an anisotropy in the electron g-tensor.

Gaining control over the g-tensor is valuable as it implies gaining control over the Zeeman splitting and therewith the spin states. For some applications it is favorable to have a nearly zero electron g-factor [22, 23], as it makes spin states robust against magnetic field fluctuations [24]. A near zero electron g-factor can be obtained by engineering the nanostructure in such a way that the spin and orbital contributions to the electron g-factor cancel each other out. The dependence of the g-tensor on size, shape and composition has been extensively investigated both theoretically and experimentally for different quantum dot systems [25, 26, 27, 28, 29, 30]. However, these parameters cannot be dynamically controlled post-growth. A scheme was proposed by Pingenot et al. [31] where the spin of a charge carrier can be fully controlled in a static magnetic field by tuning one of the components of the g-tensor around zero. This requires a method to in-situ change the electronic structure of the QD. One approach which has been investigated in the past makes use of the electric field-dependence of the g-tensor [32, 33, 34, 35, 36, 37, 38, 39], which relies on the physical displacement of the electron or hole wavefunction inside the QD. Tunability of the g-factors using electric fields is found to be limited at realistic electric field strengths and relies heavily on composition gradients in the QD.

Another approach which can be used to achieve in-situ manipulation of the electron and hole g-tensors is to induce strain in the QD structure. Strain is a powerful tool as it directly affects the band structure of the used semiconductor materials and has been passively exploited to tune the emission energy of QDs for example using lattice mismatching layers for self-assembled QDs [40] or shells around nanowire QDs [41, 42]. Active control over strain-fields can be achieved by making use of bowed airbridge structures [43, 44] or by integrating QD structures on piezoelectric actuators [45, 46, 47]. The latter approach has been used to reduce the exciton fine structure splitting and biexciton binding energy in QDs to zero [48, 49]. It is expected that externally induced strain can also be used to actively manipulate the electron and hole g-tensors, as they arise from an interplay between the different bands and strain directly affects the band structure. The work presented in this thesis extensively treats this subject for two different systems; a Zinc Blende self-assembled QD system and a Wurtzite nanowire QD system.

Under normal conditions most III-V semiconductors occur in the Zinc Blende
Chapter 1. Introduction

(ZB) crystal symmetry, which is cubic. Under specific growth conditions nanowires can be grown in the Wurtzite (WZ) crystal structure instead [50], which is hexagonal. This change in crystal structure has significant implications for the band structure. For instance, III-V semiconductors with an indirect band gap in the ZB crystal structure are predicted to have a direct band gap in the WZ crystal structure [51] and for most materials this has experimentally been established as well. Anisotropy in the spin-orbit interaction leads to a splitting between the heavy and light hole bands which are degenerate in ZB materials. While ZB materials require an anisotropic confining potential to introduce anisotropy in the g-tensor, this occurs naturally in WZ materials due to the hexagonal crystal structure. Furthermore, a WZ material and its band structure will respond differently to external stress than a ZB material, which may lead to a different behavior of the electron and hole g-tensors.

While ZB III-V semiconductors have been extensively studied and are well understood, this is certainly not true for their WZ counterparts due to their relative novelty. Work on the magnetic field dependence of WZ nanowires or QDs defined within them is limited and many parameters which are required to model these structures are unknown. The work in this thesis aims to expand the knowledge of WZ materials and to paint a comparative picture between the strain-dependence of WZ and ZB.

Apart from the g-tensor, which is the main focus of the work presented in this thesis, an externally applied magnetic field also affects the energy states in a QD via a diamagnetic contribution. The magnetic field induces a circulating current in the QD which carries a magnetic moment which couples back to the applied magnetic field. This results in an energy shift which depends quadratically on the magnetic field and which is characterized by the diamagnetic coefficient $\alpha_d$. As the diamagnetic coefficient is proportional to the lateral extension of the electron and/or hole wavefunction in the directions perpendicular to the applied magnetic field, it can be used to probe the lateral size of the wavefunctions. It is therefore interesting from a fundamental point of view, and will be treated in this thesis.

1.1 Outline of this thesis

This thesis is structured as followed. The theoretical background regarding the band structure and strain effects is discussed in Ch. 2, as well as the $k\cdot p$-theory which forms the basis for the numerical calculations presented in subsequent chapters. This chapter will also emphasize the differences between the Zinc Blende and Wurtzite crystal structures. A description of the setups used to perform the
magneto-optical experiments presented in this thesis is given in Ch. 3. Chapter 4 introduces a numerical model based on $k \cdot p$-theory which is used to calculate the emission energy, diamagnetic coefficient and electron and hole g-tensors in a self-assembled InGaAs/GaAs QD. By changing the strain distribution in the system, the strain-dependence of the aforementioned parameters is investigated. The experimental realization of this follows in Ch. 5 where strain manipulation is achieved by integrating QDs on a piezoelectric actuator. The full g-tensor is resolved for the electron and hole separately by performing magneto-optical measurements in different orientations of the magnetic field and the results are compared with the results of the numerical calculations presented in Ch. 4. The WZ nanowire QD system is introduced in Ch. 6 where by means of a finite element method the strain distribution in an InAsP nanowire QD is calculated. A Roth-like formula is then used in the effective mass approximation to describe the behavior of the electron g-tensor. Fabrication and characterization of a device to induce uniaxial strains in nanowire QDs is described in Ch. 7, which is then used to investigate the strain-dependence of the electron and hole g-tensors. The work presented in this thesis provides valuable insight in the various mechanics that contribute to the different components of the electron and hole g-tensors in QDs and shows how the strain-dependence of the g-tensors can be exploited to achieve tunability of one component around zero, which can ultimately lead to a new method to manipulate spins.
Chapter 2

Theory
2.1 Introduction

The work presented in this thesis relies on a number of theoretical frameworks which will be discussed in this chapter. In Chs. 4 and 5 calculations and experiments performed on self-assembled quantum dots (SAQDs) are presented, which are grown in the Zinc Blende (ZB) crystal structure. Chapters 6 and 7 concern nanowire quantum dots (NWQDs), which are grown in the Wurtzite (WZ) crystal structure instead. The different crystal structures have many similarities but also distinct differences regarding the subjects discussed in this chapter.

The aim of this thesis is to investigate the strain-dependence of the electron and hole g-tensors in various nanostructures. Strain is expected to influence the electron and hole g-tensors through a modification of the band structure. The electron and hole g-tensors are experimentally determined by applying a magnetic field to the investigated nanostructures. This chapter will therefore focus on two main topics; the effect of strain on the band structure in the two different crystal structures (in bulk) and the effect of magnetic fields on electron and hole states confined to a nanostructure.

The structural details and differences of the ZB and WZ lattices will be elaborated on in Sec. 2.2. The response of the different crystal structures to external stress, which takes place via the elasticity tensor, is discussed in Sec. 2.3, where it is derived how to transform the elasticity tensor from one crystal structure to another. In Sec. 2.4 the band structures of ZB and WZ are given around the Γ-point, where most of the physics governing the work presented in this thesis takes place. The band structure around the Γ-point (and its dependence on strain) can be fully described using \( k \cdot p \)-theory (Sec. 2.5), upon which the numerical calculations presented in Ch. 4 are based.

The effect of a magnetic field on electrons and holes confined to a quantum dot can be described using the full spin Hamiltonian, which consists of a Zeeman part and an exchange part. This leads to a description of the electron and hole states as a function of magnetic field in Sec. 2.6, where the splitting of the electron and hole levels with magnetic field is given in terms of electron and hole g-factors. In Sec. 2.7 the diamagnetic contribution of the magnetic field is discussed, which leads to a shift of QD emission energy quadratic in magnetic field and can experimentally be used to probe the lateral extension of the exciton wavefunction.
2.2 Zinc Blende & Wurtzite crystal structures

In bulk, III-V semiconductors such as InAs, GaAs and InP, which are the materials used in the work presented in this thesis, are grown in the so-called Zinc Blende (ZB) crystal structure. The ZB structure belongs to the cubic crystal family and its unit cell is therefore characterized by three orthogonal lattice vectors \((a, b, c)\) each with the length of the cubic lattice constant \(a_c\). The ZB lattice consists out of two interpenetrating face centered cubic (FCC) lattices, where the second lattice is translated by a quarter of the lattice constant in all directions. The resulting structure is made up of identical tetrahedra. Translation of the second lattice by \(\frac{a}{4}\) in all directions is then equivalent to a translation of the second lattice along the 111-direction by the length of one tetrahedral bond.

A well-known example of a material exhibiting this crystal structure is diamond, where both FCC lattices consist of the same atom, namely carbon. In the case of III-V semiconductors, the two FCC lattices each contain a different atom (e.g. Indium and Arsenic), leading to the ZB crystal shown in Fig. 2.1a. The ZB lattice is represented by the \(T_d\) point group.

The wurtzite (WZ) crystal structure occurs when growing III-V semiconductor nanowires under specific growth conditions [50]. The crystal is constructed by starting from the hexagonal close packed (HCP) lattice, which, contrary to ZB, can be characterized by a set of orthorhombic lattice vectors rather than a set of orthogonal lattice vectors. The non-orthogonal lattice vectors are typically labelled \(a\) and \(b\), while the vector perpendicular to the plane spanned by \(a\) and \(b\) is typically labelled \(c\). The WZ crystal consists out of two interpenetrating HCP lattices, where the second lattice is shifted along the \(c\)-axis by the length of a tetrahedral bond.

The resulting WZ structure is shown in Fig. 2.1c and is represented by the \(C_{6v}\) point group. While the ZB lattice has a lattice constant \(a_c\) which is the same in all directions, the WZ lattice has different lattice constants in the hexagonal plane and perpendicular to it, labeled \(a_{WZ}\) and \(c_{WZ}\). For an ideal WZ crystal these lattice constants are directly related to the cubic lattice constant \(a_c\) via \(a_{WZ} = \sqrt{\frac{3}{2}} a_c\) and \(c_{WZ} = \sqrt{\frac{4}{3}} a_c\) [52]. The ratio between the two lattice constant then is \(c_{WZ}/a_{WZ} = \sqrt{\frac{3}{2}} \approx 1.633\). In reality the tetrahedral building blocks of the WZ lattice are often slightly distorted and deviations from the ideal relations are encountered [52]. Some variations occur in literature between different reported values for the lattice constant caused mainly by differences in growth quality. In Table 2.1 the ideal WZ lattice constants for the two WZ materials used in the work presented in this thesis, InAs and InP, are compared with experimentally known
Figure 2.1: a) Zinc Blende and c) Wurtzite crystal structures. b) Tetrahedra along the 111-direction of a ZB crystal. d) Tetrahedra along the c-direction of a WZ crystal.
lattice constants obtained from Refs. [52] and [53]. The non-distorted predictions differ less than 0.5% from the experimental values.

On first glance the ZB and WZ crystal structures appear quite different, however their similarities become clear when considering the ZB crystal along the 111-direction as depicted in Fig. 2.1b. This image makes it clear that the ZB lattice consists of identical tetrahedra stacked in an ABC sequence. The cross-section of WZ along the c-axis as shown in Fig. 2.1d reveals that the WZ lattice is built out of the same tetrahedra, however they are stacked in an ABAB sequence and are therefore present in two different orientations. This will later be used to derive a transformation of the elasticity tensor from ZB to WZ.

Symmetry groups

Both the ZB and WZ lattices can be described by a finite set of symmetry operations. These sets of symmetry operations are represented by the $T_d$ and $C_{6v}$ point groups respectively. The names of these point groups will be used throughout this chapter. The underlying group theory goes beyond the scope of this thesis and the reader is referred to Refs. [54] and [55] for a detailed discussion.

2.3 Elasticity tensor and response to stress

From the symmetry of the crystal structures of ZB and WZ their response to an external stress can be derived. For an arbitrary, anisotropic material the relation between stress $\sigma$ (i.e. a force applied to a material), and strain $\epsilon$ (i.e. the material’s response to this stress), is given by

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

(2.1)

where $\sigma_{ij}$ and $\epsilon_{kl}$ are the components of the second rank stress and strain tensors, $\sigma$ and $\epsilon$, and $C_{ijkl}$ are the components of the the fourth rank elasticity tensor $C$. 

<table>
<thead>
<tr>
<th>Material</th>
<th>$a_c$</th>
<th>$a_{WZ,\text{ideal}}$</th>
<th>$c_{WZ,\text{ideal}}$</th>
<th>$a_{WZ}$</th>
<th>$c_{WZ}$</th>
<th>$c/a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>InAs [52]</td>
<td>6.0583</td>
<td>4.2839</td>
<td>6.9955</td>
<td>4.2742</td>
<td>7.0250</td>
<td>1.644</td>
</tr>
</tbody>
</table>

Table 2.1: Lattice constants in the non-distorted approximation and experimentally known values for WZ InAs and InP. Small deviations from the ideal ratio $c/a \approx 1.633$ are not unusual.
Chapter 2. Theory

Voigt notation

The elasticity tensor is a fourth rank tensor with 81 components. However, due to the symmetry of this tensor at most 36 components are independent. For convenience, symmetric tensors are usually written in the Voigt notation, which will also be used in the following. A second rank tensor like the stress tensor $\sigma$ can be written in Voigt notation by first tracing the diagonal, then the right column followed by the top row back to the beginning, as is indicated by the arrow in

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix} \rightarrow \sigma = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}).$$ (2.2)

For a fourth rank tensor this procedure has to be carried out twice. For a cubic crystal in the $T_d$ point group, many components of the elasticity tensor are zero and only three independent components $C_{11}, C_{12}$ and $C_{44}$ remain [56]. The elasticity tensor is then written in Voigt notation as

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}.$$ (2.3)

Note that this Voigt notation is only used for the stress and elasticity tensors. For the strain tensor the notation is slightly different; the convention is to preserve the elastic energy density $\sim \sigma_{ij} \epsilon_{ij}$. In order to achieve this, the off-diagonal components are multiplied by two - $\epsilon = (\epsilon_{11}, \epsilon_{22}, \epsilon_{33}, 2\epsilon_{23}, 2\epsilon_{13}, 2\epsilon_{12})$.

2.3.1 Transformation to Wurtzite

As most bulk III-V semiconductors occur in the ZB crystal structure, the elastic constants for ZB materials are well known. Values for the elastic constants for most WZ materials however are not experimentally known, at least for InAs and InP, the relevant materials in this thesis. Fortunately, the WZ parameters can be approximately derived from the ZB parameters using a rather straightforward transformation due to the similarities between the two crystal structures. This transformation was elegantly derived by Martin [57, 58] and the approach and results will be summarized here.

Considering an arbitrary compound AB (e.g. A=In and B=As), both the ZB and WZ lattices consist out of the same building blocks; a regular tetrahedron
of four atoms A around a single atom B. For the ZB lattice, all tetrahedra are equivalent. This is contrary to the WZ lattice, where two different tetrahedra can be distinguished. Both of these tetrahedra can be obtained from the ZB tetrahedron via a rotation, as was already depicted in Fig. 2.1.

The transformations $R^1$ and $R^2$ of the ZB tetrahedron to the corresponding WZ tetrahedra are defined by

\[
R^1 = \frac{1}{\sqrt{6}} \begin{bmatrix} \sqrt{3} & 0 & \sqrt{3} \\ -1 & 2 & 1 \\ -\sqrt{2} & -\sqrt{2} & \sqrt{2} \end{bmatrix} \quad \text{and} \quad R^2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} R^1. \quad (2.4)
\]

The elasticity tensors $C^1$ and $C^2$ for each of the tetrahedra can then be obtained by applying the respective transformation to the cubic elasticity tensor given in Eq. 2.3;

\[
C^1_{ijkl} = R^1_{im} R^1_{jn} R^1_{ko} R^1_{lp} C^Z_{mnop}. \quad (2.5)
\]

Neglecting all interactions between the tetrahedra, the elasticity tensor for Wurtzite can simply be obtained by averaging $C^1$ and $C^2$. In Voigt notation the result is given by

\[
\mathcal{C}^W = \begin{bmatrix}
C^W_{11} & C^W_{12} & C^W_{13} & 0 & 0 & 0 \\
C^W_{12} & C^W_{11} & C^W_{13} & 0 & 0 & 0 \\
C^W_{13} & C^W_{12} & C^W_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C^W_{44} & 0 & 0 \\
0 & 0 & 0 & C^W_{44} & 0 & 0 \\
0 & 0 & 0 & C^W_{66} & 0 & 0 \\
\end{bmatrix}, \quad (2.6)
\]

where

\[
\begin{align*}
C^W_{11} &= \frac{1}{6}(3C^Z_{11} + 3C^Z_{12} + 6C^Z_{44}) \\
C^W_{12} &= \frac{1}{6}(C^Z_{11} + 5C^Z_{12} - 2C^Z_{44}) \\
C^W_{13} &= \frac{1}{6}(2C^Z_{11} + 4C^Z_{12} - 4C^Z_{44}) \\
C^W_{33} &= \frac{1}{6}(2C^Z_{11} + 4C^Z_{12} + 8C^Z_{44}) \\
C^W_{44} &= \frac{1}{6}(2C^Z_{11} - 2C^Z_{12} + 2C^Z_{44}) \\
C^W_{66} &= \frac{1}{6}(C^Z_{11} - C^Z_{12} + 4C^Z_{44})
\end{align*} \quad (2.7)
\]

The equations in 2.7 are only valid when the two differently oriented tetrahedra are independent and do not interact with one another. This is a poor assumption since the tetrahedra are physically connected to each other. Martin [57, 58] fixes this issue by introducing an internal strain (IS). The elastic energy of the strained
Table 2.2: Comparison between ZB and WZ elastic constants for InAs and InP. WZ elastic constants were obtained in three ways: from Martin’s transformation [57, 58] with and without internal strain corrections and from DFT calculations performed by Hajlaoui et al. [59]

Using this approach, the elastic constants for WZ InAs and InP can be directly calculated from their respective ZB counterparts. The result is shown in Table 2.2, where it is also compared with numerical results obtained by Hajlaoui et al. [59] from density functional theory (DFT) calculations. The analytically derived elastic constants according to Martin’s method show less than 5% discrepancy with Hajlaoui’s DFT calculations. They can therefore reliably be used.

2.3.2 Poisson ratio

Due to the structure of the elasticity tensor, applying a force in one direction will not only yield a strain in that direction, but also in the perpendicular directions. The ratio between the parallel strain $\epsilon_{||}$ and perpendicular strains $\epsilon_{\perp}$ is
characterized by the Poisson ratio $\nu$ according to

$$\nu = \frac{\epsilon_\perp}{\epsilon_\parallel}, \quad (2.10)$$

and can be directly derived from the elasticity tensor. The strain as response to a certain stress is given by

$$\epsilon = S \cdot \sigma, \quad (2.11)$$

where the compliance tensor $S$ is simply the inverse of the elasticity tensor. Taking the elasticity tensor for ZB materials and a uniaxial stress applied in the $x$-direction, $\sigma = (\sigma, 0, 0, 0, 0)$, yields a strain tensor of the form $\epsilon = (\epsilon_\parallel, \epsilon_\perp, \epsilon_\perp, 0, 0, 0)$, from which the uniaxial Poisson ratio $\nu_1$ can be calculated using Eq. 2.10;

$$\nu_1^{ZB} = \frac{C_{12}}{C_{11} + C_{12}}. \quad (2.12)$$

As the ZB lattice is cubic, this result is independent of which principal axis the stress is applied along. The Zinc Blende system described in Chs. 4 and 5 however is exposed to a biaxial stress, $\sigma = (\sigma, \sigma, 0, 0, 0, 0)$, leading to a biaxial Poisson ratio $\nu_2$

$$\nu_2^{ZB} = 2 \frac{C_{12}}{C_{11}} = \frac{2\nu_1^{ZB}}{1 - \nu_1^{ZB}}. \quad (2.13)$$

The Wurtzite system described in Chs. 6 and 7 will experience a uniaxial stress along the $c$-axis, leading to a Poisson ratio of

$$\nu^{WZ} = \frac{C_{13}}{C_{11} + C_{12}}. \quad (2.14)$$

In Chs. 4 and 6 strain profiles for different quantum dot systems are numerically calculated, with and without the application of external stress. The expressions for the Poisson ratios derived here will be used to check the accuracy of the calculated results.

### 2.4 Band structure

The similarities between the crystal structures of the ZB and WZ lattices, which were already made clear in Fig. 2.1, have important implications for the resulting band structure. To describe the physics relevant to this work only the center of the Brillouin zone, the $\Gamma$-point, needs to be considered. In general, it is sufficient to take into account only the bottom conduction band and top three valence bands, which are all two-fold degenerate due to spin for a total of eight bands. For ZB materials these bands are well-known. Electrons occupying the bottom
Chapter 2. Theory

Heavy hole (HH)
Light hole (LH)
Conduction (CB)
Split-off (SO)

Conduction (CB)
Heavy hole (HH)
Light hole (LH)
Crystal field split (CH)

6
8
7
7
9
7
7

Zinc Blende (ZB) Wurtzite (WZ)
Band gap

Figure 2.2: Band diagrams of Zinc Blende and Wurtzite materials at the Γ-point.

The conduction band (CB) have an $s$-like character with orbital momentum $L = 0$ and the band belongs to the $\Gamma_6$ representation of the $T_d$ double group. The valence band has a $p$-like character with $L = 1$. Due to the non-zero orbital momentum, the valence band is heavily affected by the spin-orbit coupling, which couples the spin of a charge carrier to the magnetic field induced by its own orbital motion. As a result, for the valence band the orbital momentum $L$ is no longer a clean quantum number. Instead, the valence band is characterized by the total angular momentum $J = L + S$, which is either $\frac{3}{2}$ or $\frac{1}{2}$. The valence bands with $J = \frac{1}{2}$ ($\Gamma_7$) are split-off (SO) from the bands with $J = \frac{3}{2}$ ($\Gamma_8$) by the spin-orbit energy $\Delta_{so}$. In bulk semiconductors the bands with $J = \frac{3}{2}$ are degenerate at the Γ-point and can be divided into heavy holes (HH) and light holes (LH) according to the $z$-projection $J_z$ of the total angular momentum, which is $\frac{3}{2}$ for the heavy hole and $\frac{1}{2}$ for the light hole. The band structure at the Γ-point for ZB is sketched in Fig. 2.2.

For the WZ structure the situation is quite similar. The most significant deviation from the ZB band structure originates from the reduced symmetry of the WZ crystal. Not taking into account spin-orbit coupling, the hexagonal crystal field of the WZ lattice splits off the heavy and light hole bands formed by $p_x$ and $p_y$ orbitals from the crystal field split hole band (CH) formed by $p_z$ orbitals by the crystal field energy $\Delta_{cf}$. When including the spin-orbit interaction, this splitting increases. The spin-orbit interaction also induced a splitting between the heavy and light hole bands. The heavy hole then becomes the top-most valence band,
Chapter 2. Theory

State | Zinc Blende | Wurtzite
--- | --- | ---
CB $\uparrow$ | $\Gamma_6, +\frac{1}{2}$ | $\Gamma_{7v}, +\frac{1}{2}$
CB $\downarrow$ | $\Gamma_6, -\frac{1}{2}$ | $\Gamma_{7v}, -\frac{1}{2}$
HH $\uparrow$ | $\Gamma_8, \frac{3}{2}$ | $\Gamma_{9v}, \frac{3}{2}$
HH $\downarrow$ | $\Gamma_8, -\frac{3}{2}$ | $\Gamma_{9v}, -\frac{3}{2}$
LH $\uparrow$ | $\Gamma_8, \frac{1}{2}$ | $\Gamma_{7v}, +\frac{1}{2}$
LH $\downarrow$ | $\Gamma_8, -\frac{1}{2}$ | $\Gamma_{7v}, -\frac{1}{2}$
SO $\uparrow$ | $\Gamma_7, +\frac{1}{2}$ | $\Gamma_{7v}, +\frac{1}{2}$
SO $\downarrow$ | $\Gamma_7, -\frac{1}{2}$ | $\Gamma_{7v}, -\frac{1}{2}$

Table 2.3: Basis functions for the eight most important bands for the Zinc Blende and Wurtzite crystal symmetries. For the $\Gamma_{7v}$ bands in Wurtzite, $a$ and $b$ are material dependent normalization constants which follow from $k\cdot p$-theory.

followed by the light hole and crystal field split hole bands. The bands belong to the $\Gamma_9$, $\Gamma_7$ and again $\Gamma_7$ representations of the $C_{6v}$ double group respectively [51]. For materials which have a direct band gap in the ZB phase, such as InP and InAs, the lowest conduction band in the WZ phase belongs to the $\Gamma_7$ representation. The band structure at the $\Gamma$-point for WZ is sketched in Fig. 2.2. In general, the band gap for WZ materials is slightly larger than the band gap for their ZB counterparts.

2.4.1 Basis functions

The bands in Fig. 2.2 can be characterized by the basis functions of their corresponding irreducible representations. These basis functions are always linear combinations of the $s$-like conduction band state $|s\rangle$ and the $p$-like valence band states $|x\rangle$, $|y\rangle$ and $|z\rangle$. The basis functions for ZB [60] and WZ [61] follow from group theory and are given in Table 2.3, where the states $|s\rangle$, $|x\rangle$, $|y\rangle$ and $|z\rangle$ and the spinors $\chi^\uparrow$ and $\chi^\downarrow$ have been replaced with $S$, $X$, $Y$, $Z$, $\uparrow$ and $\downarrow$ respectively. Note that in the case of WZ the material-dependent constants $a$ and $b$ mix the in-plane and out-of-plane $p$-orbitals. These constants arise from $k\cdot p$-theory which will be discussed in Sec. 2.5.
Chapter 2. Theory

### 2.5 $k \cdot p$-theory

In order to determine the band structure around the Γ-point or the influence of induced strain, a more sophisticated model is required. Many ways to calculate the band structure of a semiconductor material exist, like the tight-binding model, the pseudopotential approximation or $k \cdot p$-theory. The latter forms the basis for the numerical model employed in Ch. 4 and provides a valuable insight on the influence of strain on the band structure of WZ and ZB materials. Its main advantage is the fact that it relies solely on simple zone-center parameters, which can easily be determined experimentally or estimated theoretically.

The theory is derived by combining the Schrödinger equation with Bloch’s theorem. In its most general form, the time-independent Schrödinger equation is given by

\[ H |\Psi\rangle = E |\Psi\rangle, \quad (2.15) \]

where $|\Psi\rangle$ is the eigenstate of the system, $E$ its corresponding eigenenergy and $H$ the Hamiltonian describing the system. For the simple case of a single particle, the Hamiltonian is given by

\[ H = \left( \frac{p^2}{2m} + V(r) \right), \quad (2.16) \]

where $p = -i\hbar \nabla$ is the momentum operator, $m$ is the effective mass of the particle, $r$ is the position vector and $V(r)$ is the potential describing the system. Combining this with Bloch’s theorem forms the basis for $k \cdot p$-theory. Bloch’s theorem states that the wavefunction $\psi(r)$ in a periodically-repeating environment, such as a semiconductor crystal, can be expressed as the product of a plane wave $e^{i k \cdot r}$, where $k$ is the wave vector, and a fast oscillating periodic function $u(r)$ with the same periodicity as the crystal lattice according to

\[ \psi_{n,k}(r) = e^{i k \cdot r} u_{n,k}(r) \quad (2.17) \]

where $\psi_{n,k}(r)$ are solutions of Eq. 2.16 and $n$ is the band index denoting the respective band. Combining Eqs. 2.15, 2.16 and 2.17 leads to

\[ H u_{n,k} = \left( \frac{p^2}{2m} + \frac{\hbar k \cdot p}{m} + \frac{\hbar^2 k^2}{2m} + V(r) \right) u_{n,k} = E_{n,k} u_{n,k}. \quad (2.18) \]

The $k \cdot p$-term, which gives name to the theory, originates from the differential part of the momentum operator. The $k$-independent part in Eq. 2.18 represents the Hamiltonian $H_0$ at the center of the Brillouin zone where $k = 0$. The solutions $u_{n,0}$ of

\[ H_0 u_{n,0} = \left( \frac{p^2}{2m} + V(r) \right) u_{n,0} = E_{n,0} u_{n,0} \quad (2.19) \]
will form a complete and orthonormal set of basis functions with which the crystal is described. The \( k \)-dependent terms can then be treated as a perturbation.

### 2.5.1 Including spin-orbit interaction

Since the spin-orbit interaction plays a major role in the behaviour of the band structure, it should be included in the Hamiltonian. The Hamiltonian for the spin-orbit interaction \( H_{so} \) is given by [54]

\[
H_{so} = \frac{\hbar}{4c^2m^2}(\nabla V \times p) \cdot \sigma,
\]

where \( c \) is the speed of light and \( \sigma \) is the Pauli vector containing the Pauli matrices given by

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

This leads to a new Hamiltonian for which Eq. 2.18 has to be solved [60];

\[
H = H_0 + H_k + H_{kp} + H_{so} + H'_{so}.
\]

where

\[
H_0 = \frac{p^2}{2m} + V(r),
\]

\[
H_k = \frac{\hbar^2k^2}{2m},
\]

\[
H_{kp} = \frac{\hbar k \cdot p}{m},
\]

\[
H_{so} = \frac{\hbar}{4m^2c^2}(\nabla V) \times p \cdot \sigma
\]

and \( H'_{so} = \frac{\hbar^2}{4m^2c^2}(\nabla V) \times k \cdot \sigma \).

### 2.5.2 Strain-dependent \( k \cdot p \)-Hamiltonian

The Hamiltonian given in Eq. 2.23 is valid in the absence of strain. The ZB Hamiltonian including strain used in the calculations was derived by Bahder [60, 62] by introducing a modified crystal potential and restoring the periodicity of the unstrained crystal via a coordinate transformation.

The full Hamiltonian is given in Ref. [60] and includes terms caused by the lack of inversion symmetry of the crystal. Usually, these terms are neglected as they are small and insignificant. This results in a slightly simplified eight-band Hamiltonian. In the ZB basis described in Table 2.3, the strain-independent Hamiltonian is given by
Chapter 2. Theory

\[
\begin{pmatrix}
A & 0 & \sqrt{3}V & -\sqrt{2}U & -U & \sqrt{2}V^* \\
0 & A & -\sqrt{2}U & -\sqrt{3}V^* & 0 & -V & \sqrt{2}V \\
V & -\sqrt{2}U & -P + Q & -S^* & R & 0 & \sqrt{3}S - \sqrt{2}Q \\
0 & -\sqrt{3}V & -S & -P - Q & 0 & R & -\sqrt{2}R \frac{1}{2} \sqrt{2}S \\
\sqrt{3}V^* & 0 & R^* & 0 & -P - Q & S^* & \frac{1}{2} \sqrt{2}S^* \sqrt{2}R^* \\
-\sqrt{2}U & -V^* & 0 & R^* & S & -P + Q & \sqrt{2}Q \sqrt{3}S^* \\
-\sqrt{2}V^* & \sqrt{2}V^* & \sqrt{3}S^* & -\sqrt{2}R^* & \frac{1}{2} \sqrt{2}S & \sqrt{2}Q & Z & 0 \\
\sqrt{2}V & U & -\sqrt{2}Q & \frac{1}{2} \sqrt{2}S & \sqrt{2}R & \sqrt{3}S & 0 & Z \\
\end{pmatrix}
\] (2.24)

where

\[
A = E_c + (F + \frac{\hbar^2}{2m_0})(k_x^2 + k_y^2 + k_z^2),
\]
\[
U = \frac{1}{\sqrt{3}} P_0 k_z,
\]
\[
V = \frac{1}{\sqrt{6}} P_0 (k_x - ik_y),
\]
\[
P = -E_v + \frac{1}{2} \gamma_1 \frac{\hbar^2}{m_0} (k_x^2 + k_y^2 + k_z^2),
\]
\[
Q = \frac{1}{2} \gamma_2 \frac{\hbar^2}{m_0} (k_x^2 + k_y^2 + k_z^2),
\]
\[
R = -\sqrt{3 \frac{\hbar^2}{2m_0}} (\gamma_2 (k_x^2 - k_y^2) - 2 \nu \gamma_3 k_x k_y),
\]
\[
S = \sqrt{3 \gamma_3} \frac{\hbar^2}{m_0} k_z (k_x - ik_y),
\]
\[
Z = E_v - \Delta - \frac{1}{2} \gamma_1 \frac{\hbar^2}{m_0} (k_x^2 + k_y^2 + k_z^2).
\] (2.25)

Here \(E_c\) and \(E_v\) are the conduction band and valence band energies respectively. \(\Delta\) represents the spin-orbit coupling, while \(P_0\) is the momentum matrix element coupling the valence band to the conduction band. \(F\) describes the mixing of the conduction band with remote bands. Finally, \(\gamma_1, \gamma_2\) and \(\gamma_3\) are modified Luttinger parameters. Note that all off-diagonal elements are \(k\)-dependent, such that at the \(\Gamma\)-point \((k_x = k_y = k_z = 0)\) only the diagonal elements remain. The eigenvalues at zone center are then given by \(E_c\) (twofold), \(E_v\) (fourfold) and \(E_v - \Delta\) (twofold).
The strain-dependent part is given by

\[
\begin{pmatrix}
\alpha' e & 0 & -v^* & 0 & -\sqrt{3}v & \sqrt{2}u & u & -\sqrt{2}v^* \\
0 & \alpha' e & \sqrt{2}u & \sqrt{3}v^* & 0 & v & -\sqrt{2}v & u \\
-v & \sqrt{2}u & -p + q & -s^* & r & 0 & \sqrt{3} s & -\sqrt{2}q \\
0 & \sqrt{3}v & -s & -p - q & 0 & r & -\sqrt{2}r & \frac{1}{2}\sqrt{2}s \\
-\sqrt{3}v^* & 0 & r^* & 0 & -p - q & s^* & \frac{1}{2}\sqrt{2}s^* & \sqrt{2}r^* \\
\sqrt{2}u & v^* & 0 & r^* & s & -p + q & \sqrt{2}q & \sqrt{3} s^* \\
u & -\sqrt{2}v^* & \sqrt{3} s^* & -\sqrt{2}r^* & \frac{1}{2}\sqrt{2}s & \sqrt{2}q & -ae & 0 \\
-\sqrt{2}v & -u & -\sqrt{2}q & \frac{1}{2}\sqrt{2}s^* & \sqrt{2}r & \sqrt{3} s^* & 0 & -ae
\end{pmatrix}
\]  

(2.26)

where

\[
w = \frac{1}{\sqrt{3}} b' \epsilon_{xy},
\]

\[
p = a (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}),
\]

\[
t = \frac{1}{\sqrt{6}} b' (\epsilon_{xz} + \epsilon_{yz}),
\]

\[
q = b (\epsilon_{zz} - \frac{1}{2} (\epsilon_{xx} + \epsilon_{yy})),
\]

\[
u = \frac{1}{\sqrt{3}} P_0 \sum_j \epsilon_{zj} k_j,
\]

\[
r = \frac{\sqrt{2}}{2} b (\epsilon_{xx} - \epsilon_{yy}) - id \epsilon_{xy},
\]

\[
v = \frac{1}{\sqrt{6}} P_0 \sum_j (\epsilon_{xj} - \epsilon_{yj}) k_j,
\]

\[
s = -d (\epsilon_{xz} - \epsilon_{yz}),
\]

\[
e = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz},
\]

and \(a, a', b\) and \(d\) are deformation potentials. From inspection of the diagonal elements of the strain-dependent heavy hole - light hole submatrix

\[
\begin{pmatrix}
-p + q & -s^* & r & 0 \\
-s & -p - q & 0 & r \\
r^* & 0 & -p - q & s^* \\
0 & r^* & s & -p + q
\end{pmatrix}
\]  

(2.28)

it is clear that hydrostatic strain (i.e. \(\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}\)) does not change the symmetry of the system and \(q = 0\), protecting the degeneracy of the heavy hole and light hole bands. However, the heavy hole and light hole bands will split-up when exposed to a non-hydrostatic strain. In the case of QDs the strain configuration is usually such that the heavy hole band becomes the top valence band.
Several $k \cdot p$-models for Wurtzite structures exist [63, 64, 65]. The most commonly used model is the Hamiltonian derived by Chuang and Chang [61]. This model uses the WZ basis functions listed in Table 2.3, without the mixing between the in-plane and out-of-plane orbitals in the $\Gamma_7v$ valence bands (i.e. $a = 0, b = 1$). The strain-independent Hamiltonian at the $\Gamma$-point is given by

\[
\begin{pmatrix}
E_c & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & E_c & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & E_{v+} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & E_{v+} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & E_{v-} & 0 & 0 & \sqrt{2}\Delta_3 \\
0 & 0 & 0 & 0 & 0 & E_{v-} & \sqrt{2}\Delta_3 & 0 \\
0 & 0 & 0 & 0 & 0 & \sqrt{2}\Delta_3 & E_v & 0 \\
0 & 0 & 0 & 0 & 0 & \sqrt{2}\Delta_3 & 0 & E_v
\end{pmatrix}
\] (2.29)

where $E_{v+} = E_v + \Delta_1 + \Delta_2$ and $E_{v-} = E_v + \Delta_1 - \Delta_2$. In the quasi-cubic approximation $\Delta_{1,2,3}$ can be related to the crystal field splitting $\Delta_{cf}$ and the spin-orbit splitting $\Delta_{so}$ via

\[
\Delta_1 = \Delta_{cf}, \quad \Delta_2 = \Delta_3 = \frac{\Delta_{so}}{3}.
\] (2.30)

The off-diagonal components in the bottom-right block of the WZ Hamiltonian then lead to mixing between the different $\Gamma_7v$ valence band states. These off-diagonal components also lead to more complicated expressions for the band edge energies compared to the ZB case. The band edge energies at the $\Gamma$-point are given by

\[
E_c, \\
E_1 = E_v + \Delta_1 + \Delta_2, \\
E_2 = E_v + \frac{\Delta_1 - \Delta_2}{2} + \sqrt{\left(\frac{\Delta_1 - \Delta_2}{2}\right)^2 + 2\Delta_3^2}, \\
E_3 = E_v + \frac{\Delta_1 - \Delta_2}{2} - \sqrt{\left(\frac{\Delta_1 - \Delta_2}{2}\right)^2 + 2\Delta_3^2}.
\] (2.31)

Their corresponding eigenfunctions are the basis functions previously given in Table 2.3. The equations in Eq. 2.31 immediately show the splitting between the heavy hole and light hole bands in absence of strain.
Chuang and Chang also derived the strain-dependent Hamiltonian, from which the strain-dependent band edge energies at $k = 0$ follow analytically. For the derivation and full Hamiltonian the reader is referred to Ref. [61]. The result is given by

$$E_{\epsilon}^c = E_0^c + \Delta_1 + \Delta_2 + E_g + a_{czz} \epsilon_{zz} + a_{ct}(\epsilon_{xx} + \epsilon_{yy}),$$
$$E_{\epsilon}^1 = \Delta_1 + \Delta_2 + \theta_\epsilon + \lambda_\epsilon,$$
$$E_{\epsilon}^2 = \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon + \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2}\right)^2 + 2\Delta_3^2},$$
$$E_{\epsilon}^3 = \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon - \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2}\right)^2 + 2\Delta_3^2}.$$  \hspace{1cm} (2.32)

where

$$\lambda_\epsilon = D_1 \epsilon_{zz} + D_2 (\epsilon_{xx} + \epsilon_{yy}),$$
$$\theta_\epsilon = D_3 \epsilon_{zz} + D_4 (\epsilon_{xx} + \epsilon_{yy}),$$  \hspace{1cm} (2.33)

and $a_{czz}$, $a_{ct}$, $D_1$, $D_2$, $D_3$ and $D_4$ are deformation potentials which define the dependence of the band edges on strain. The normalization constants $a$ and $b$, which mix the second and third valence bands are given by

$$a = \frac{2\Delta_3^2}{\sqrt{(E_{\epsilon}^c - \lambda_\epsilon)^2 + 2\Delta_3^2}}, \quad b = \frac{E_{\epsilon}^c - \lambda_\epsilon}{\sqrt{(E_{\epsilon}^c - \lambda_\epsilon)^2 + 2\Delta_3^2}}.$$  \hspace{1cm} (2.34)

### 2.6 Spin Hamiltonian

Throughout this thesis, different nanostructures will be exposed to an external magnetic field. This magnetic field will couple to the intrinsic magnetic moment, better known as spin, of the electrons and holes confined in the nanostructures. Experimentally the electron and hole are not measured independently, but rather in the form of a Coulomb-coupled pair called an exciton. In order to analyze the behaviour of these excitons in an external magnetic field, the full spin Hamiltonian has to be considered, which consists out of two parts; a Zeeman Hamiltonian and an electron-hole exchange Hamiltonian. Since for QDs exhibiting either the Wurtzite or the Zinc Blende crystal structure the heavy hole band is the top most valence band, and in the strained heterostructures discussed in this thesis the separation from the light hole band is generally large, the discussion can be limited to excitons consisting of an electron with $S_z = \frac{1}{2}$ and a heavy hole with $J_z = \frac{3}{2}$. This leads to four possible exciton states, characterized by their total angular momentum projections $M = \pm 1$ or $M = \pm 2$. These exciton states are then used as a basis to construct the exchange and Zeeman Hamiltonians. Only the exciton states with $M = \pm 1$ are optically active and therefore called bright excitons. The other
two states with $M = \pm 2$ are then logically referred to as dark excitons. The full description is given in Ref. [66] and the results are summarized here.

### 2.6.1 Exchange Hamiltonian

The electron-hole exchange interaction is a quantum mechanical effect which arises from the condition that for fermions the total wavefunction of a many-particle state is anti-symmetric under the exchange of spatial coordinates and spin. The exchange Hamiltonian $H_{\text{exchange}}$ was derived by van Kesteren et al. [67] for the $T_d$ double group of Zinc Blende crystals and is given by

$$H_{\text{exchange}} = - \sum_{i=x,y,z} (a J_{h,i} S_{e,i} + b J_{h,i}^3 S_{e,i})$$

(2.35)

where $a$ and $b$ are spin-spin coupling constants. In the following the heterostructure growth direction is chosen to be parallel to the $z$-direction. Using the exciton states with a total angular momentum projection $M = S_{e,z} + J_{h,z} = \pm 1, \pm 2$ as a basis, the exchange Hamiltonian can be expressed as

$$H_{\text{exchange}} = \frac{1}{2} \begin{bmatrix} \delta_0 & \delta_1 & 0 & 0 \\ \delta_1 & \delta_0 & 0 & 0 \\ 0 & 0 & -\delta_0 & \delta_2 \\ 0 & 0 & \delta_2 & -\delta_0 \end{bmatrix}.$$

(2.36)

where $\delta_0 = \frac{3}{2} a_z + \frac{27}{8} b_z$, $\delta_1 = \frac{3}{4} (b_x - b_y)$ and $\delta_2 = \frac{3}{4} (b_x + b_y)$. From the block diagonal form of Eq. 2.36 it is evident that no mixing between the bright and dark exciton states occurs. The bright excitons are split from the dark excitons by the electron-hole exchange energy $\delta_0$. The bright excitons themselves are split by the fine structure splitting (FSS) $\delta_1$, which is zero for heterostructures with a rotational invariance. The dark excitons are split by the FSS $\delta_2$, which is non-zero.

**Charged excitons**

Besides the straightforward neutral exciton consisting of one electron and one hole, excitonic complexes consisting of more than two charge carriers can also occur. The positively and negatively charged trions consisting out of one electron and two holes or two electrons and one hole do not exhibit any exchange interaction. This is evident when considering for example the negatively charged trion as a hole interacting with a spin-singlet electron pair. The observed spectrum depends on both the initial state of the exciton and the final state after recombination. In this case the final state is a single electron which cancels out the exchange splitting of the trion and it is not observed in the emission.
Biexciton

Another excitonic complex which is commonly observed in the heterostructures discussed throughout this thesis is the biexciton, consisting out of a spin-singlet hole pair interacting with a spin-singlet electron pair. Since the biexciton itself does not exhibit any exchange splitting and the final state is a neutral exciton which does exhibit exchange splitting, the observed emission also shows an exchange splitting.

The different excitonic complexes usually differ a few meV in emission energy due to the Coulomb interaction. Depending on the exact size, shape and composition of the QD, the ordering and spacing of the different excitonic peaks observed in a photoluminescence spectrum varies. Each QD therefore has a unique PL spectrum, which can be used as a fingerprint to identify a QD. This property is heavily exploited in the work presented in this thesis, to find the same QD from experiment to experiment.

2.6.2 Zeeman Hamiltonian

The interaction of an externally applied magnetic field $B$ with arbitrary orientation and magnitude with electron and hole spins is given by [67]

$$H_{Zeeman}(B) = -\mu_B \sum_i (g_{e,i} s_{e,i} - 2\kappa_i J_{h,i} - 2q_i J_{h,i}^3) B_i,$$  \hspace{1cm} (2.37)

where $\mu_B$ is the Bohr magneton, $s_{e,i}$ and $J_{h,i}$ are the electron and hole spins respectively, and $q_i$ and $\kappa_i$ are the valence band parameters in the Luttinger-Kohn Hamiltonian [68, 69]. Again since only the heavy hole is considered, the simplification $J_h = \frac{3}{2}$ can be used. The structure of the Zeeman Hamiltonian depends heavily on the direction of the applied magnetic field. Here the two most relevant orientations will be discussed; $B$ parallel to the growth direction (Faraday geometry) or $B$ perpendicular to the growth direction (Voigt geometry).

Faraday geometry

In the Faraday geometry the magnetic field is aligned with the growth direction of the QD ($B = (0, 0, B_z)$). Substituting $J_{h,z}^2 = \frac{9}{4}$ and $g_{h,z} = 6\kappa_z + \frac{27}{2}q_z$ [66] in Eq. 2.37 then leads to the Faraday Hamiltonian

$$H_F = \frac{\mu_B B_z}{2} \begin{bmatrix}
ge_{e,z} + g_{h,z} & 0 & 0 & 0 \\
0 & -g_{e,z} - g_{h,z} & 0 & 0 \\
0 & 0 & -g_{e,z} + g_{h,z} & 0 \\
0 & 0 & 0 & g_{e,z} - g_{h,z}
\end{bmatrix}. \hspace{1cm} (2.38)$$
In absence of exchange splitting the situation is then straightforward; the two bright excitons are separated by $\mu_B(g_{e,z} + g_{h,z})B_z$, while the dark excitons are separated by $\mu_B(g_{e,z} - g_{h,z})B_z$. Due to the optical selection rules, only the bright excitons are visible and emit right-handed circularly polarized ($\sigma_+$) and left-handed circularly polarized ($\sigma_-$) light.

The exchange interaction can be included by simply summing the two Hamiltonians of Eqs. 2.36 and 2.38. Diagonalization of the resulting Hamiltonian leads to the energies given by

\begin{align}
E_1 &= \frac{1}{2}\delta_0 + \frac{1}{2}\sqrt{\delta_1^2 + (g_e + g_h)^2\mu_B^2 B^2}, \\
E_2 &= \frac{1}{2}\delta_0 - \frac{1}{2}\sqrt{\delta_1^2 + (g_e + g_h)^2\mu_B^2 B^2}, \\
E_3 &= -\frac{1}{2}\delta_0 + \frac{1}{2}\sqrt{\delta_2^2 + (g_e - g_h)^2\mu_B^2 B^2}, \\
E_4 &= -\frac{1}{2}\delta_0 - \frac{1}{2}\sqrt{\delta_2^2 + (g_e - g_h)^2\mu_B^2 B^2}.
\end{align}

**Voigt geometry**

In the Voigt geometry the magnetic field is applied perpendicular to the QD growth direction. Here the $x$-axis is chosen, leading to the Voigt Hamiltonian

\[ H_V = \frac{\mu_B B_x}{2} \begin{bmatrix} 0 & 0 & g_{e,x} & g_{h,x} \\
0 & 0 & g_{h,x} & g_{e,x} \\
g_{e,x} & g_{h,x} & 0 & 0 \\
g_{h,x} & g_{e,x} & 0 & 0 \end{bmatrix}. \]

The off-diagonal block form of the Voigt Hamiltonian mixes the bright states with the dark states, causing all states to be visible. Combining this with the exchange Hamiltonian from Eq. 2.36 yields the eigenenergies

\begin{align}
E_1 &= +\frac{1}{4}(+\delta_1 + \delta_2 + \sqrt{(2\delta_0 + \delta_1 - \delta_2)^2 + 4\mu_B^2(g_e - g_h)^2 B^2}), \\
E_2 &= +\frac{1}{4}(-\delta_1 - \delta_2 + \sqrt{(2\delta_0 - \delta_1 + \delta_2)^2 + 4\mu_B^2(g_e + g_h)^2 B^2}), \\
E_3 &= -\frac{1}{4}(+\delta_1 + \delta_2 + \sqrt{(2\delta_0 - \delta_1 + \delta_2)^2 + 4\mu_B^2(g_e + g_h)^2 B^2}), \\
E_4 &= -\frac{1}{4}(-\delta_1 - \delta_2 + \sqrt{(2\delta_0 + \delta_1 - \delta_2)^2 + 4\mu_B^2(g_e - g_h)^2 B^2}).
\end{align}

**Arbitrary angle**

Due to the absence of the dark states in the Faraday geometry, a measurement with the magnetic field at an angle in between the two different configurations is
necessary to determine the full g-tensor for the electron and hole separately. From
Eq. 2.37 it is clear that the Zeeman Hamiltonian in this intermediate configuration is merely a linear combination of the Faraday and Voigt Hamiltonians. An
arbitrary magnetic field applied under an angle \( \beta \) with the nanostructure growth
direction \( \mathbf{B} = (\sin \beta, 0, \cos \beta) B_0 \) then leads to

\[
H_Z = \frac{\mu_B B_0}{2} \begin{bmatrix}
    b(g_{e,z} + g_{h,z}) & 0 & a_{e,x} & a_{h,x} \\
    0 & b(-g_{e,z} - g_{h,z}) & a_{g,h,x} & a_{g,e,x} \\
    a_{g,e,x} & a_{g,h,x} & b(-g_{e,z} + g_{h,z}) & 0 \\
    a_{g,h,x} & a_{g,e,x} & 0 & b(g_{e,z} + g_{h,z})
\end{bmatrix}.
\] (2.42)

where \( a = \sin \beta \) and \( b = \cos \beta \). Adding the exchange Hamiltonian from Eq.
2.36 and subsequent diagonalization leads to the eigenenergies, which can still
be solved analytically but no longer produces simple and insightful equations for
the eigenenergies. Only when disregarding the exchange interaction, manageable
equations are obtained as

\[
E = \frac{\mu_B B_0}{2} \left( \pm \sqrt{(g_{h,x} \sin \beta)^2 + (g_{h,z} \cos \beta)^2} \pm \sqrt{(g_{e,x} \sin \beta)^2 + (g_{e,z} \cos \beta)^2} \right).
\] (2.43)

**A note on Wurtzite**

The derivation presented above was originally performed for the \( T_d \) double group
to which Zinc Blende crystals belong. However, the symmetry arguments made
in the derivations are also valid for the Wurtzite crystal structure. Therefore
the exchange and Zeeman Hamiltonian will have the same shape and symmetry,
although the analytical values of the coefficients may be different. The latter is not
relevant, since in this thesis the exchange splittings and g-factors are determined
experimentally.

### 2.7 Diamagnetic shift

An external magnetic field affects the energy states not only through the Zeeman
effect but also through the diamagnetic shift. Apart from the intrinsic magnetic
moment which gives rise to the Zeeman effect, application of an external mag-
netic field induces an orbital motion of the electron, i.e. a circular current, which
has a magnetic moment as well. This magnetic moment then couples back to
the magnetic field, which causes an energy shift known as the diamagnetic shift.
Analogous to the classical case of a simple current loop, where the magnitude of
the magnetic moment is determined by the area over which it extends, one might
already suspect the magnitude of this diamagnetic shift to depend on the lateral size of the considered nanostructure, since this defines the extension of the orbital motion of the electron, i.e. its wavefunction.

The diamagnetic shift for a single charge carrier confined to a QD can be understood when considering a harmonic oscillator potential,

\[ V_{QD} = \frac{1}{2} m^* (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (2.44) \]

where \( m^* \) is the effective mass of the charge carrier and \( \omega_{x,y,z} \) are the eigenfrequencies in the three orthogonal directions. Assuming cylindrical symmetry of the dot \( \omega_x = \omega_y \) when taking the \( z \)-axis as the quantization axis of the QD. The solutions to the harmonic oscillator potential are well known [70] and the ground state is given by

\[ E_0 = \frac{1}{2} \hbar \omega_x + \frac{1}{2} \hbar \omega_y + \frac{1}{2} \hbar \omega_z = \hbar \omega_{x,y} + \frac{1}{2} \hbar \omega_z. \quad (2.45) \]

Inclusion of an external magnetic field leads to a slight adjustment which was derived by Darwin [71] and Fock [72]. Applying a magnetic field in the \( z \)-direction merely leads to an additional orbital motion in the \( xy \)-plane and is incorporated in the ground state energy via the cyclotron frequency, \( \omega_c = \frac{qB}{m^*} \). This results in the Fock-Darwin energies, of which the ground state is given by [73]

\[ E = \hbar \sqrt{\frac{\omega_c^2}{4} + \omega_{x,y}^2} + \frac{1}{2} \hbar \omega_z. \quad (2.46) \]

Defining the magnetic length \( l_B = \sqrt{\frac{\hbar}{m^* \omega_c}} \) and lateral extension length \( l_{x,y} = \sqrt{\frac{\hbar}{2m^* \omega_{x,y}}} \) this can be written as

\[ E = \frac{\hbar^2}{2m^* l_{x,y}^2} \sqrt{1 + \frac{l_{x,y}^4}{l_B^4}} + \frac{1}{2} \hbar \omega_z. \quad (2.47) \]

At a typical magnetic field strength of 1 T the magnetic length is approximately 26 nm, which is larger than the typical lateral extension length of the wavefunction limited by the size of the QD. A Taylor expansion can therefore be used to approximate Eq. 2.47 which, upon resubstituting the magnetic length, results in

\[ E = E_0 + \frac{e^2 l_{x,y}^2}{8 m^*} B^2 = E_0 + \alpha_d B^2, \quad (2.48) \]

where \( \alpha_d = \frac{e^2 l_{x,y}^2}{8 m^*} \) is the diamagnetic coefficient. The diamagnetic shift depends quadratically on the applied magnetic field. Furthermore, the diamagnetic coefficient also scales with the lateral extension of the charge carriers wavefunction. As
a consequence, the diamagnetic shift can be used directly as a probe to determine the size of the charge carrier’s wavefunction. The inverse dependence on the effective mass also shows the diamagnetic shift of an electron is expected to be higher than the diamagnetic shift of a hole.

2.7.1 Extension to excitons

When considering an electron-hole pair rather than a single charge carrier, a first approach would be to simply sum the two separate diamagnetic coefficients to obtain the diamagnetic coefficient for the exciton. This is a valid approach when the electron and hole are separated far from each other and the Coulomb interaction is weak. In general the diamagnetic coefficient for an exciton in a quantum disk, a quantum dot with a high aspect ratio such as the ones discussed in this thesis, is given by [74, 75, 76]

\[
\alpha_d = \frac{e^2}{8\mu} < \rho^2 >,
\]

(2.49)

where \(\mu\) is the reduced exciton mass defined by \(\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}\) and \(< \rho^2 >\) is the average effective exciton radius in the plane perpendicular to the applied magnetic field. Again this is only valid for small magnetic fields, where the exciton radius is smaller than the magnetic length. For high magnetic fields, the diamagnetic shift depends linearly on the applied magnetic field instead [77].
Chapter 2. Theory
Chapter 3

Experimental techniques
3.1 Introduction

Throughout this thesis photoluminescence experiments are performed on different QD systems to gain information about the electronic structure of the QDs. Often this is combined with high magnetic fields to specifically investigate the Zeeman splitting and diamagnetic shift. The vast majority of the experiments presented in this thesis are performed using two different setups which will be discussed in this chapter; the characterization setup (Sec. 3.2) and the magneto-luminescence setup (Sec. 3.3).

3.2 Characterization setup

It is often helpful to be able to quickly check the quality and performance of a certain sample or device. For this a characterization setup is used, which is a rather simple free-space photoluminescence setup. The setup contains a Helium flow cryostat to cool down the sample to 4 K. The cryostat is mounted on a translation stage for rough positioning and contains internal stepper motors for fine positioning of the sample with respect to the objective, which is mounted right above it. The used objective is designed for the NIR range (480-1800 nm), and, with a magnification of 100x, focuses a fiber-coupled laser to a spot with a size of ± 1 μm. Light emitted by the sample or device mounted in the cryostat is picked up by the same objective and, via a beamsplitter placed above the objective, directed
towards a spectrometer for wavelength analysis. An additional beamsplitter in the excitation path allows for the sample and laser spot to be imaged on a camera. The setup is schematically shown in Fig. 3.1.

The spectrograph is an Acton sp2500i and contains three different gratings with 300, 600 and 1200 grooves per millimeter, corresponding to a pixel-to-pixel distance of roughly 180, 80 and 30 \( \mu \text{eV} \) at 950 nm. In practice the resolution of the spectrometer is limited by the width of the entrance slit and the alignment of the camera with respect to the grating, yielding optimal resolutions of roughly twice the pixel-to-pixel distance. The PL is finally detected by a Silicon charge coupled device (CCD).

3.3 Magneto-luminescence setup

In order to determine the electron and hole g-tensors of bulk semiconductors or nanostructures, in this thesis photoluminescence experiments are performed in the presence of high magnetic fields. The magnetoluminescence setup used to perform these experiments consists out of four elements; the cryostat, the insert, the optical head and the spectrometer. The whole system is schematically described in Fig. 3.2 and the components will be discussed one by one.

3.3.1 The cryostat

The setup contains a bath cryostat which can be filled with 35 liters of liquid Helium, allowing for the system to be kept at a temperature of 4 K for two days without refilling. A superconducting magnet is located at the bottom of the helium bath, capable of applying magnetic fields up to 10 T along the cryostat axis. The bath contains temperature sensors at two different places to monitor the temperature of the system.

The cryostat possesses two vacuum shields; the outer vacuum shield isolates the cryostat from its surroundings while the inner vacuum shield can be used to isolate the insert from the Helium bath. Since in this case both the magnet and sample need to be cooled down to 4 K, the inner vacuum shield is not used but instead filled with a low pressure of helium gas.

3.3.2 The insert

The insert is a long metal tube which is inserted into the cryostat. The sample stage is located at the bottom of this insert in such a way that the sample experiences a maximal and homogeneous magnetic field. The sample stage con-
sists of one Attocube piezoelectric z-positioner (ANPz51) and two x-positioners (ANPx51) designed for vacuum systems and cryogenic temperatures for full control over the position of the sample. The presence of a resistive encoder allows the position to be readout with a sub $\mu$m accuracy. The sample is mounted on top of the stack of piezoelectric positioners. The objective located directly above the sample has a working distance of 1.6 mm. The magnetic field can only be applied in one direction. Therefore to change the geometry of the experiment, i.e. to apply the magnetic field in a different direction with respect to the sample, both the sample and the objective have to be rotated. To achieve this, a small periscope containing three beamsplitters and an objective can be installed. The final beamsplitter and objective are rotatable, allowing for any angle of illumination (and collection) with respect to the applied magnetic field. Different sample mounts are available to mount the sample under different angles correspondingly.

### 3.3.3 The optical head

The optical head is placed on top of the insert and contains, apart from the objective which is located in the insert, all necessary optics to perform the experiments.

For most experiments presented in this thesis a Thorlabs S1FC635 fiber-coupled
laser source with an excitation wavelength of 635 nm is used, which enters the optical head through a fiber connected to the excitation arm. The PL emitted by the sample is eventually coupled out of the optical head via a fiber connected to the collection arm. The excitation and collection arms are identical to one another and both fibers are single mode and angle polished to reduce internal reflections. In both the arms there is space to mount polarization optics for polarization dependent measurements.

In between the arms a number of optical elements is crucial to ensure maximum efficiency in both excitation and collection of the PL. In both arms the fiber is mounted in a Thorlabs SM1Z z-translation stage right behind a Thorlabs C220TMD-B aspheric lens. This allows for precise adjustment of the focus to produce a collimated beam in the excitation arm, or efficient coupling into the fiber in the collection arm. Both arms are mounted on a Thorlabs ST1XY-D xy-translation stage for alignment purposes.

The arms are connected via a Thorlabs M254H45 hot mirror with a cutoff wavelength of 700 nm. The hot mirror has high transmission (>90 %) below 700 nm and high reflectance (>95 %) above 700 nm. Since typically an excitation wavelength of 635 nm is used, while the investigated structures emit between 800 and 1000 nm, this ensures maximum efficiency in both excitation and collection of the photoluminescence. For other purposes the hot mirror can easily be replaced with an ordinary beam splitter.

An additional beamsplitter is added to the excitation arm to be able to image the laser spot on a camera. This is essential to align the optical head and to navigate the laser spot across the sample. Due to the long distance (±2 meters) it is not feasible to illuminate the sample in such a way that the sample itself can be imaged. Therefore localization of the nanostructures on the sample is performed solely on basis of the reflected laser spot.

The entire optical head is mounted on a Thorlabs KC1-T tilt plate to be able to direct the excitation beam through the center of the objective. Finally, the hot mirror is mounted on a Thorlabs B4CRP rotatable mount which contains three additional screws to adjust the tip, tilt and height of the hot mirror. This provides sufficient degrees of freedom to achieve efficient incoupling of the PL into the single mode collection fiber. Furthermore, once performed, the internal alignment of the optical head is stable to such extent that PL signal of a quantum dot is not lost after refilling the system with helium. When removing and replacing the optical head, only the tilt plate has to be used for re-alignment.
3.3.4 The spectrometer

The spectrometer is an Acton sp7500i, similar to the one used with the characterization setup. It has a focal length of 75 cm and contains three different gratings of 750, 1100 and 1800 grooves per mm. The first two gratings have a blazing designed for the near infrared, while the latter one has a blazing designed for the visible spectrum. The non-ideal blazing angle has consequences for the detected PL intensity, which is reduced by roughly a factor five at a wavelength of 900 nm. Unfortunately this grating is used most for the experiments, since accurate determination of the Zeeman splitting requires an as high as possible resolution. The dispersed PL signal is detected by a Si CCD. Xenon, Neon and Argon lamps are available for calibration of the spectrometer.
Chapter 4

Numerical calculations of a strained self-assembled quantum dot

Parts of this chapter were adapted from:

Chapter 4. Numerical calculations of a strained self-assembled quantum dot

4.1 Introduction

This chapter will present numerical calculations on a self-assembled quantum dot. These calculations are performed to support the experiments presented in Ch. 5. In these experiments a piezoelectric actuator is used to apply a compressive in-plane biaxial stress to self-assembled InGaAs QDs. The application of external stress will induce strain in the QDs which affects the electronic structure, emission energy, diamagnetic coefficient and g-tensors. The experiments are performed in magnetic fields up to 10 T to determine the g-tensor for both the electron and hole, and how they vary with the induced strain. In order to understand the physical mechanisms underlying these experiments, a numerical model based on $k\cdot p$-theory is employed.

This chapter discusses this numerical model and the results obtained with it. First a brief overview of the numerical model will be given in Sec. 4.2 followed by a discussion of the strain calculations in Sec. 4.3. The results from the strain calculations are used as an input for the electronic calculations without an external magnetic field in Sec. 4.4 and with an external magnetic field in Sec. 4.5. Finally an analysis of the strain dependence of the g-tensors and the diamagnetic coefficients is given in Secs. 4.6 and 4.7.

4.2 Details of the numerical model

The numerical model was developed by Craig Pryor at the University of Iowa [78, 79] and is based on the eight-band $k\cdot p$-model described in Sec. 2.5 using the Hamiltonians in Eqs. 2.24 and 2.26. The model allows the calculation of the electronic structure for any given nanostructure and can incorporate external magnetic fields to compute g-factors.

Throughout the entire chapter the numerical model is applied to a lens-shaped In$_{0.4}$Ga$_{0.6}$As dot with a radius of 10 nm and a height of 2.5 nm, embedded in a GaAs matrix. These parameters are representative for the QDs investigated in the experiment.

The model places the desired structure on a cubic grid and assigns the required material parameters to each grid site. The QD growth axis is defined as the $z$-direction. Material parameters are taken from Ref. [80] for T=0. Parameters for composite materials, such as the QD material In$_{0.4}$Ga$_{0.6}$As, are determined by linear interpolation between the components (Vegard’s law), except when Ref. [80] provides bowing parameters (for $E_g$, $\Delta$, $\gamma_3 - \gamma_2$, $E_p$, $E_v$ and $a_c$.) Then continuum elasticity theory is used to compute the strain at each point. Typically
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

A 200×200×200 grid with a spacing of 0.5 nm is used. This suffices for the strain to be fully relaxed at the border of the grid, which is required due to the periodic boundary conditions.

The electronic calculations are then performed on the same grid, using the acquired strain as an input. Usually the grid is truncated to a smaller size before this step, as the exponential decay of the wavefunctions into the host material eliminates the necessity for the large grid that was used for the strain calculations. Truncation of the grid greatly increases the computation speed for the electronic calculations. Depending on the confinement of the electron and hole, which determines the extension of their wavefunctions, usually an area of 20 nm around the QD suffices for the electronic calculations. Derivatives of the envelope functions are replaced by finite differences on the grid, which results in a large sparse Hamiltonian which is then diagonalized using the Lanzcos algorithm. In this way the energies of the electron and hole states and their wavefunctions are obtained.

Finally, g-factors and diamagnetic coefficients can be determined by repeating the computation in the presence of a uniform magnetic field, which couples to both the spin and orbital moment [20, 81]. Spurious midgap states [82, 83] are eliminated by including an optimized second-nearest-neighbour term [84].

4.3 Strain calculations

Due to the lattice mismatch between GaAs and In$_{0.4}$Ga$_{0.6}$As, which is roughly 2.8 %, a compressive strain is already present in the system without applying any external stress. In the experiments presented in Ch. 5 an in-plane biaxial stress will be applied to the QDs. The influence of this can be mimicked by introducing an additional layer of an artificial material under the structure in the computational grid, which from now on will be referred to as the stressor. Varying the lattice constant of this stressor has the same effect as biaxially applying external stress perpendicular to the QD growth direction and results in additional strain in the QD and its surrounding GaAs barrier. To ensure that all strain is incorporated in the QD-barrier system rather than in the stressor layer, the elastic constants ($C_{11}$, $C_{12}$ and $C_{44}$) in the stressor layer are set to unphysically large values. This forces the stressor to be rigid, while only the QD-barrier system reacts to stress.

Choosing the lattice constant of the stressor to be the same as of GaAs yields a situation where no external stress is applied. The top row in Fig. 4.1 then shows the components of the resulting strain tensor on two cross-sectional planes of the QD; The $xy$-plane through the bottom of the QD (i.e. the ground plane) and the $xz$-plane through the center of the QD. The strain components in the plane of the
Figure 4.1: Components of the strain tensor on cross-sectional planes through the dot when no strain is added (top row), when 1% compressive strain is added (middle row) and the difference between the two (bottom row).

<table>
<thead>
<tr>
<th>Difference</th>
<th>-1% external strain</th>
<th>No external strain</th>
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quantum dot, $\epsilon_{xx}$ and $\epsilon_{yy}$ are near the 2.8 % compressive strain which is to be expected from the lattice mismatch. The strain in the growth direction, $\epsilon_{zz}$, is tensile rather than compressive. This can be understood by considering the high aspect ratio of the QD, which causes the Poisson effect to force the strain in the $z$-direction to compensate the strong compressive strain in the $xy$-plane.

Choosing the lattice constant of the stressor to be 1 % smaller than the lattice constant of the GaAs barrier results in the strain profiles shown in the middle row of Fig. 4.1. Comparing them with the external stress-free situation depicted in the top row, no substantial change in the strain profiles is observed apart from an offset. This is emphasized by showing the difference between the two situations in the bottom row of Fig. 4.1. Averaged over the dot, the additional strain induced by varying the lattice constant of the stressor layer by 1 %, is 0.99 % for the $x$- and $y$-components of the strain tensor, $\epsilon_{xx}$ and $\epsilon_{yy}$. Since in the $xy$-plane of the QD $\epsilon_{xx}$ and $\epsilon_{yy}$ are identical apart from a rotation of 90°, it can be concluded that the induced strain is indeed biaxial. The strain induced by the stressor layer is fully transferred to the QD. Furthermore, the strain is affected as good as homogeneously. Only at the edges of the QD deviations are found, however they are limited to at most 0.03 %. Discretization of the grid induces some artefacts close to the edge of the QD, which are especially well visible for the $z$-component of the strain, $\epsilon_{zz}$. The increase in compressive strain in the $xy$-plane is accompanied by an increase in tensile strain in the growth direction of the QD by 0.97 %, leading to a Poisson ratio of 0.98. In Sec. 2.3.2 it was derived that the biaxial Poisson ratio for Zinc Blende materials $\nu^ZB$ is given by

$$\nu^ZB = 2 \frac{C_{12}}{C_{11}} \quad (4.1)$$

and using elastic constants for the QD material In$_{0.4}$Ga$_{0.6}$As obtained by interpolating between the experimentally known elastic constants for GaAs ($C_{11} = 122.1 \text{ GPa}, C_{12} = 56.6 \text{ GPa}$ [80]) and InAs ($C_{11} = 83.29 \text{ GPa}, C_{12} = 45.26 \text{ GPa}$ [85]) yields a biaxial Poisson ratio of 0.98, the same value which follows from Fig. 4.1. Note that the values for the elastic constants listed by Vurgaftman in Ref. [80] are actually off by a factor of ten due to an erroneous translation of units. This however does not have any consequences for the calculation of strain profiles, as this merely depends on ratios between elastic constants which are obviously still correct.
4.4 Electronic calculations

The previously calculated strain profile is used as an input for the electronic calculations, where it immediately affects the band structure through the strain-dependent part of the \( \mathbf{k} \cdot \mathbf{p} \)-Hamiltonian. This is illustrated in Fig. 4.2a, where the conduction and valence band edges are plotted along a line across the ground plane of the QD when only the built-in strain from the lattice mismatch is present (solid lines) and when 1\% of biaxial compressive strain is induced (dashed lines). The shifts of the bottom conduction band edge and the top valence band edge are plotted in b) for the center of the QD (in black) and a point in the GaAs host far away from the QD where the built-in strain is relaxed (in red). c) Splitting between the heavy hole and light hole bands inside the QD.

Figure 4.2: a) Band edges on a line across the ground plane of the QD when only the built-in strain from lattice mismatch is present (solid lines) and when 1\% biaxial compressive strain is induced (dashed line). The shifts of the bottom conduction band edge and the top valence band edge are plotted in b) for the center of the QD (in black) and a point in the GaAs host far away from the QD where the built-in strain is relaxed (in red). c) Splitting between the heavy hole and light hole bands inside the QD.
band gap increase in the InGaAs dot (≈4.4 meV). For both the electron in the conduction band and the hole in the valence band the barrier is effectively raised.

In the unstressed case, the strain caused by the lattice mismatch between the dot and the host is relaxed within 10 nm outside the dot and no strain is present in the GaAs host beyond this point. Because of this, the heavy hole and light hole bands are degenerate in the GaAs host. Adding 1 % compressive strain to the system lifts this degeneracy. At the same time the heavy hole and light hole bands in the QD, which were already split due to the lattice mismatch between the InGaAs QD and the GaAs host, split up even further. This is illustrated in Fig. 4.2c, where the splitting between the two bands increases from 117 meV to 120 meV at $\Delta \epsilon_{||} = -0.1 \%$.

Note that for the strain calculations and the calculation of the band structure results up to 1 % were shown to emphasize the effects of strain. As the amount of strain which is achieved in the experiment presented in Ch. 5 is much lower, for the remainder of this chapter a maximum of $\Delta \epsilon_{||} = -0.1 \%$ is used.

Finally the electron and hole ground states are calculated. This yields the emission energy of the QD, which is shown in Fig. 4.3. The emission energy of the QD increases by 4.65 meV at $\Delta \epsilon_{||} = -0.1 \%$, which is similar to the band gap increase in the QD of 4.4 meV.

### 4.5 Magnetic field

In order to compute g-factors and diamagnetic shifts, an external magnetic field has to be incorporated in the calculations. The result is shown in Fig. 4.4, where
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

Figure 4.4: Left: splitting of the electron and hole ground states as a function of magnetic field, for magnetic fields applied in the plane of the dot (in black) and in the growth direction of the dot (in red). Right: Zeeman splittings and diamagnetic shifts as a function of magnetic field for each ground state in both orientations of the magnetic field. The diamagnetic coefficients given in the figure are in $\mu\text{eV/T}^2$.

The energies of the electron and hole ground states are plotted for magnetic fields up to 10 T applied parallel and perpendicular to the QD growth direction. The growth axis is defined along the $z$-direction. Due to the cylindrical symmetry of the QD applying a magnetic field in the $x$-direction is equivalent to applying one in the $y$-direction. The $y$-direction is therefore omitted from the rest of the discussion, and only g-factors and diamagnetic coefficients along $x$ (in-plane) and $z$ (out-of-plane) are given. From the Zeeman splitting at high magnetic fields it is clear that the out-of-plane hole g-factor $g_{h,x}$ is much larger than all other components. The diamagnetic shift for the electron is much larger than for the hole. To further illustrate this, the second part of Fig. 4.4 shows the Zeeman splitting of each ground state and the average energy of each ground state (i.e. the diamagnetic shift) as a function of the applied magnetic field. The Zeeman
splitting follows the expected linear behaviour perfectly, while the diamagnetic shift can be accurately fit with a quadratic dependence. Since this is the case, it suffices to perform the rest of the calculations for only one given magnetic field. In this case 10 T is chosen.

The sign of the g-factors is defined in such a way that when a magnetic field is applied along a certain axis and the state with a negative total momentum projection onto this axis is the ground state, the g-factor is considered to be positive [86]. The sign of the diamagnetic coefficient is defined to be positive for the electron as well as the hole.

### 4.6 Strain-dependence of the g-tensors

The out-of-plane and in-plane components of the electron and hole g-tensors can now be calculated when varying the amount of strain induced in the system, the result of which is shown in Fig. 4.5. For each component the slope of the fitted line, which gives the change in g-factor per percent of induced strain, is given in Table 4.1. In Ch. 5 these calculations will be accompanied by experimental results. In the experiment the g-factor is determined per meV change in emission energy rather than strain. In order to compare between the two, in the final column of Table 4.1 the slope is divided by the tunability of the emission energy as obtained from Fig. 4.3.

The most sensitive component is the out-of-plane hole g-factor $g_{h,z}$, with a sensitivity ten times larger than the next most sensitive component $g_{e,x}$. The in-plane hole g-factor $g_{h,x}$, which is nearly zero, is virtually unaffected. The opposite is true for the electron, where the in-plane component $g_{e,x}$ is more sensitive compared to the out-of-plane component $g_{e,z}$.

Since every wavefunction is a superposition of the Bloch states of all bands, the exact value of the g-factors originates from an interplay between those bands. Therefore the composition of the electron and hole ground states has to be considered. Furthermore, the confinement of the wavefunctions will quench the orbital momentums associated with the g-factors and has therefore to be taken into account. The electron and hole will be discussed separately.

#### 4.6.1 Electron

The out-of-plane and in-plane electron g-factors have quite similar values, being $g_{e,z} = -0.057$ and $g_{e,x} = 0.171$ respectively. The small anisotropy between the two is later explained in terms of the quenching of the orbital momentum. Both components increase when adding strain to the system, however the magnitude
Figure 4.5: Calculated electron and hole g-factors for the in-plane and out-of-plane directions as a function of the added strain.

Table 4.1: Values of the g-factors and their sensitivities to strain determined from the numerical calculations. In the last column the sensitivities are divided by the sensitivity of the emission energy to obtain a quantity which can more easily be compared to the experiments presented in Ch. 5.

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
<th>$dg/d\Delta\varepsilon_{\parallel}$</th>
<th>$dg/dE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{h,z}$</td>
<td>-2.582</td>
<td>-2.349</td>
<td>50.516</td>
</tr>
<tr>
<td>$g_{h,x}$</td>
<td>-0.102</td>
<td>-0.017</td>
<td>0.366</td>
</tr>
<tr>
<td>$g_{e,z}$</td>
<td>-0.057</td>
<td>-0.062</td>
<td>1.333</td>
</tr>
<tr>
<td>$g_{e,x}$</td>
<td>0.171</td>
<td>-0.264</td>
<td>5.677</td>
</tr>
</tbody>
</table>

of the increase is quite different between the two. The in-plane electron g-factor $g_{e,x}$ is much more sensitive to the added strain than the out-of-plane g-factor $g_{e,z}$. To gain insight into the origin of the increase of the electron g-factors and their anisotropy, two separate contributions which cause the electron g-factor to deviate from the free electron value of 2 need to be considered: the mixing of the valence band into the electron ground state and the quenching of the orbital momentum.
Valence band mixing

Spin-orbit coupling causes a (negative) deviation from the spin g-factor of 2 [9], according to

\[ g_e = 2 - g_{orb}. \]  \( (4.2) \)

However, since the conduction band is made up of s-orbitals which do not have an angular momentum, it does not contribute to the orbital part of the g-factor. A pure conduction band state would therefore have \( g_{orb} = 0 \), leading to a g-factor of 2. However, in the eight-band model the electron ground state wavefunction is a superposition of the eight Bloch states which form the basis for the \( k \cdot p \)-Hamiltonians in Sec. 2.5 rather than a pure conduction band state. Due to the coupling between the conduction band and the valence band, the valence bands mix into the electron ground state. The \( p \)-states of the valence band, which have a non-zero angular momentum, then lead to a non-zero \( g_{orb} \).

When investigating the composition of the wavefunction, it is found that the electron ground state wavefunction has 96.16 % conduction band character. The remainder is made up of the valence band (2.16 % light hole, 0.96 % split-off and 0.72 % heavy hole). The composition of the electron ground state wavefunction for various amounts of induced strain is shown in Fig. 4.6a. At \( \Delta \epsilon_\parallel = -0.1 \% \), the amount of CB character decreases by 0.03 %. This change is negligible and contradicts the observed behavior, especially for the in-plane component \( g_{e,x} \), as it would lead to an increase of the VB contribution and therewith a decrease in the electron g-factor. This can therefore be ruled out as the main mechanism behind the observed strain-sensitivity.

Orbital momentum quenching

As mentioned earlier, the orbital contribution to the magnetic moment (and hence the g-factor) originates from the spin-orbit interaction which gives rise to spin-correlated currents. By lifting orbital degeneracies, the confining potential limits the coherent mixing of different orbital states and therefore decreases the contribution of the orbital current to the magnetic moment. This mechanism is referred to as orbital angular momentum quenching [20, 21]. In the presence of an applied magnetic field the current induced by this magnetic field contributing to the magnetic moment is perpendicular to the field and therefore the g-factor will be affected by the confinement transverse to the applied field.

Asymmetry in the confining potential leads to anisotropy in the angular momentum quenching, and hence in the g-factor. Such anisotropy has for example been observed in InAs/InP QDs [17, 19]. With a radius \( r \) that is much larger than
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

Figure 4.6: Composition of the electron and hole ground states in absence of a magnetic field as a function of the added strain. Note which component belongs to which axis, as indicated by the arrows.
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

the height $h$, the dots described in this chapter deviate significantly from spherical
symmetry, however the g-factor is less anisotropic than in Ref’s [17] and [19]. The
weak anisotropy seen in the calculations presented here indicates electrons in these
dots are weakly confined to the QD, as will be verified later.

The barrier height does not alone determine the confinement strength. For
example, a nominally high barrier will provide only weak confinement if the well is
so small that the energy of the confined state is close to the energy of the barrier
material. For this reason, it is advantageous to evaluate the degree of confinement
by examining the wave function and its penetration into the barrier material. The
lateral extension of the electron wavefunction is affected by strain in two ways.
Firstly, biaxial compressive strain will decrease the dot radius and through the
Poisson effect increase the height of the dot. This effect is relatively small as the
maximum strain used in the calculations is only $\Delta \epsilon_\parallel = -0.1 \%$ and can therefore
be neglected. More importantly, strain shifts the edge of the conduction band,
which will consequently affect the degree of confinement of the electron state in
the dot. From the $k\cdot p$-Hamiltonian in Eq. 2.26 follows that the shifts of the
conduction band edge with strain is given by $\Delta E_c = a_c \epsilon$, where $a_c$ is the material
specific hydrostatic deformation potential and $\epsilon = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$ is the trace of
the strain tensor. For the biaxial compressive strain dealt with in this system,
$\epsilon$ is negative. The values of $a_c$ for GaAs and InAs are -7.17 eV and -5.08 eV
respectively, resulting in a larger increase of the conduction band edge for the
GaAs barrier compared to the InGaAs dot, as was already shown in Fig. 4.2b.
This effectively raises the barrier and the electron is more strongly confined. This
effect has been confirmed experimentally on similar dots, where it has been shown
to give rise to an increase of the biexciton binding energy upon compression [49].

To further illustrate this, Fig. 4.7 shows the probability density $|\psi|^2$ for both
the electron and hole on the ground plane and the $xz$-plane through the center
of the dot. It is evident that the electron shows weaker confinement compared to
the hole. Especially in the growth direction, the leaking into the GaAs barrier
is significant. By integrating $|\psi_e|^2$ over the dot material, it is found that roughly
50 % of the probability density of the wavefunction is accommodated in the barrier
rather than the dot. Figure 4.8b shows how this develops when adding strain. The
part of the probability density that is confined inside the dot increases by roughly
1 % when $\Delta \epsilon_\parallel = -0.1 \%$ and can directly be related to the confinement energy as
shown on the right axis since both quantities show a linear dependence on strain.
The confinement energy is given by the energy difference between the electron
ground state and the conduction band edge of the surrounding barrier as depicted
in Fig. 4.8a. To conclude, due to an increase in electron confinement, the extension
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

Figure 4.7: Probability density ($|\psi_{e,h}|^2$) on the ground plane and the $xz$-plane through the center of the dot for both the electron (a) and (b)) and the hole (c) and (d)). The solid white line indicates the edge of the QD. The probability density in each figure has been normalized to the maximum value to allow for a better comparison.

of the electron wavefunction into the surrounding GaAs barrier decreases, leading to a smaller orbital contribution and an increase in (the quenching of) the electron $g$-factor. As the leaking of the wavefunction into the barrier is more pronounced in the growth direction, the in-plane electron $g$-factor $g_{e,x}$ is most affected.

4.6.2 Hole

The out-of-plane hole $g$-factor $g_{h,z}$ has a value of -2.582 and is extremely sensitive to the added strain, with a sensitivity that is 10 times higher than the sensitivity of the in-plane electron $g$-factor $g_{e,x}$. The in-plane hole $g$-factor $g_{h,x}$ on the other hand has a value close to zero, -0.102, and is virtually unaffected by the added
Figure 4.8: Probability density integrated over the QD volume for both b) the electron and c) the hole as a function of the added strain. On the right axis the corresponding confinement energy, which is indicated in a), is given.

While for the electron the barrier has to be taken into account, this is not the case for the hole. Figures 4.7c and 4.7d show the hole is confined well within the dot. Integration of $|\psi_h|^2$ over the dot materials shows that roughly 85 % of the hole ground state wavefunction is confined in the dot, which changes by only 0.15 % at $\Delta \epsilon_\parallel = -0.1$ % added strain as shown in Fig. 4.8c. Counter-intuitively this is accompanied by a small decrease in the confinement energy from 128.6 meV to 128.3 meV. The confinement energy of the hole is much larger than the confinement of the electron which explains why it is more localized inside the dot material. Due to the large fraction of the probability density located in the dot and the relatively small change with added strain, only the contribution of the dot itself has to be considered. Unfortunately, the complex nature of the valence band makes an intuitive approach for the hole g-factor impossible. Where the electron g-factor has a clear limit of 2 for infinite quenching, for the hole g-factor such a constant limit does not exist [86]. However, with some simple arguments the sensitivity of the hole g-factor can at least qualitatively be explained.
Due to the symmetry of the dot \((r \gg h)\), the dominating character in the ground state hole wavefunction is the heavy hole, contributing more than 94\%. The orbital momentum of the HH Bloch state only has a projection along the \(z\)-axis. A pure HH state would therefore have \(g_{h,x} = 0\) and \(g_{h,z} \neq 0\). This explains the large anisotropy between the values of the in-plane and out-of-plane hole g-factors that is observed in the calculation.

As the hole g-factor experiences a large shift in the out-of-plane direction, the composition of the ground state must be sensitive to the applied strain. To illustrate this, the calculated contribution of each of the bands to the ground state hole wavefunction is shown in Fig. 4.6b.

The contribution from both the conduction band and split-off band is negligible and not sensitive to the added strain. The heavy hole contribution increases by 0.25\% which is entirely compensated by an equal decrease in the light hole contribution. Previous research has already shown that the hole g-factor is extremely sensitive to this exact composition [25, 26]. This therefore qualitatively explains the observed shift. In case of the in-plane hole g-factor \(g_{h,x}\), strain is affecting something that is close to zero, so in absolute terms the change is small.

### 4.7 Diamagnetic shift

Apart from the g-tensor, the electron and hole are also affected by the diamagnetic shift. The diamagnetic shift arises from the orbital motion induced by the magnetic field, which is characterized by a magnetic moment which couples back to the magnetic field. The diamagnetic shift \(E_{dia} = \alpha_d B^2\) depends quadratically on the magnetic field.

Since the diamagnetic shift follows a perfect quadratic dependence on magnetic field as was illustrated in Fig. 4.4, the diamagnetic coefficients for the electron and hole \(\alpha_{d,e,h}\) can be extracted from the calculations using only the energies at 0 T, \(E_{0,e,h}\), and 10 T, \(E_{1,2,e,h}|_{B=10}\), according to

\[
\alpha_{d,e,h} = \frac{E_{1,e,h}|_{B=10} + E_{2,e,h}|_{B=10}}{2B^2} - \frac{E_{0,e,h}}{B^2}. \tag{4.3}
\]

In this case both the electron and hole diamagnetic coefficients are defined to be positive and the exciton diamagnetic coefficient is given by the sum of the two.

The diamagnetic coefficients for the electron and hole are calculated for magnetic fields applied both in-plane and out-of-plane for various amounts of induced strain and the result is shown in Fig. 4.9.
Chapter 4. Numerical calculations of a strained self-assembled quantum dot

Figure 4.9: In-plane (in red) and out-of-plane (in black) diamagnetic coefficients for a) the electron and b) the hole as a function of strain. The strain-dependence of the diamagnetic coefficients is compared to the strain-dependence of the spread of the wavefunction in the various directions by the dashed lines.

According to Eq. 2.48 the diamagnetic coefficient of either the electron or hole is given by

$$\alpha_d = \frac{e^2}{8} \frac{l^2}{m^*}$$  \hspace{1cm} (4.4)

where $m^*$ is the effective mass and $l$ is the extension of the wave function perpendicular to the applied magnetic field. The diamagnetic coefficients for the hole, which have values of $\alpha_{d,z}^{h,z} = 0.99 \, \mu eV/T^2$ and $\alpha_{d,x}^{h,x} = 0.17 \, \mu eV/T^2$ are an order of magnitude smaller than the diamagnetic coefficients for the electron, which have values of $\alpha_{d,z}^{e,z} = 8.2 \, \mu eV/T^2$ and $\alpha_{d,x}^{e,x} = 4.1 \, \mu eV/T^2$. This is caused by a larger effective mass and a smaller lateral extension of the wavefunction for the hole compared to the electron. For both the electron and the hole, $\alpha_{d}^{x}$ is significantly larger than $\alpha_{d}^{z}$. This is easily explained by considering the high aspect ratio of the QD, since the diamagnetic coefficient depends on the lateral extension of the wavefunction perpendicular to the direction of the applied magnetic field. This anisotropy is commonly observed in self-assembled QDs [25, 87].

**Electron**

The diamagnetic coefficients for the electron for the different directions of the magnetic field, which are shown in Fig. 4.9a, both decrease as a function of strain. Similar to the electron g-factor, the diamagnetic coefficient is mostly determined by the lateral extension of the wavefunction and therefore closely connected to the confinement of the electron in the conduction band. Because under the influence of strain the electron is more strongly confined, which consequently decreases
the lateral extension of the wavefunction, the diamagnetic coefficients decrease with increasing strain. The in-plane diamagnetic coefficient is relatively much more strongly affected than the out-of-plane diamagnetic coefficient, decreasing by respectively 4.1 % and 1.4 % at $\Delta \epsilon_{||} = -0.1 \%$. This anisotropy is analogous to the previously observed anisotropy in the sensitivity of the electron g-factor.

The leakage of the electron wavefunction into the surrounding host is the most prominent along the growth direction of the QD, which causes the lateral extension of the electron wavefunction in that direction to be most strongly affected by strain. This results in a more sensitive diamagnetic coefficient when the magnetic field is applied perpendicular to the QD growth direction.

The effect of strain on the lateral extension of the electron wavefunction can be quantified by considering the spread of the wavefunction in the $x$, $y$- and $z$-directions $\sigma_{x,y,z}$, defined by $\sigma_{x}^2 = \langle x^2 \rangle - \langle x \rangle^2$. This serves as a good measure for the lateral extension of the wavefunction and is numerically calculated by

$$\sigma_{x}^2 = \sum_{n} x^2 |\psi|^2 - (\sum_{n} x|\psi|^2)^2$$

where $n$ sums over all grid sites. For the electron $\sigma_{x}^e = \sigma_{y}^e = 4.0 \text{ nm}$ and $\sigma_{z}^e = 2.5 \text{ nm}$. Since the diamagnetic coefficient scales with $\sigma^2$, it is worthwhile to investigate how much $\sigma_{x,y}^2$ and $\sigma_{z}^2$ are relatively affected by strain and compare this with the strain-dependence of the diamagnetic coefficients. It is found that $\sigma_{z}^2$ and $\sigma_{x,y}^2$ decrease by respectively 4.5 % and 1.3 % at $\Delta \epsilon_{||} = -0.1 \%$, corresponding well with the relative decreases of 4.1 % and 1.4 % that were found for the diamagnetic coefficients. This is illustrated by the dashed lines in Fig. 4.9a, where $\sigma_{x}^2$ and $\sigma_{x,y}^2$ have been normalized to the corresponding diamagnetic coefficients. This shows that for the electron the relative changes in $\sigma_{z}^2$ and $\sigma_{x,y}^2$ closely follow the relative changes in the diamagnetic coefficients. The strain-dependence of the diamagnetic coefficients can therefore be ascribed to the effect of strain on the confinement and the lateral extension of the electron wavefunction.

**Hole**

Figure 4.9b shows the strain-dependence of the hole diamagnetic coefficients. Both increase as a function of strain, however in absolute sense the sensitivity is negligible compared to the sensitivity of the diamagnetic coefficients for the electron. In the experiment in Ch. 5 the exciton diamagnetic coefficient is determined, which is given by the sum of the electron and hole diamagnetic coefficients. Both the value and the strain-dependence of the exciton diamagnetic coefficient are therefore dominated by the electron, and the influence of the hole can be disregarded in the experiment.
Nonetheless it is interesting to investigate the strain-dependence of the diamagnetic coefficients of the hole the same way as was done for the electron. The lateral extension of the hole is calculated to be $\sigma_{x}^{h} = \sigma_{y}^{h} = 3.0$ nm and $\sigma_{z}^{h} = 0.9$ nm. Especially in the growth direction this is much smaller than $\sigma_{z}^{e} = 2.5$ nm which was found for the electron, as is expected due to the better localization of the hole wavefunction compared to the electron wavefunction. As is indicated by the dashed lines in Fig. 4.9b, the change of the diamagnetic coefficients of the hole cannot be explained by considering the lateral extension of the wavefunction alone. It is therefore likely that the origin of the strain-dependence of the diamagnetic coefficients for the hole lies in the effective mass, as this is the only other parameter contributing to $\alpha_{d}$.

4.8 Conclusions

This chapter has presented numerical calculations performed using an eight-band $k \cdot p$-model to investigate the dependence of the electron and hole g-tensors in a typical InGaAs QD on induced strain. Strain is induced in the entire computational grid by introducing a stressor layer at the bottom of the grid and varying its lattice constant. The resulting biaxial strain is fully understood by considering the Poisson effect.

The electronic calculations show a linear dependence of the electron and hole energy levels on the induced strain. When introducing an external magnetic field, both the Zeeman splitting and diamagnetic shift show their expected (respectively linear and quadratic) dependence on magnetic field.

When determining the electron and hole g-tensor as a function of induced biaxial strain it is found that the out-of-plane hole g-factor is by far the most sensitive component, which is understood by considering the effect of the heavy hole-light hole splitting on the composition of the hole ground state wavefunction. The much smaller change in electron g-factors is explained in terms of the effect of the confinement energy on the size of the wavefunction. The experimentally determined exciton diamagnetic coefficient, which is given by the sum of the electron and hole separately, is dominated by the electron. The diamagnetic coefficients were calculated and compared to the lateral size of the wavefunctions. For the electron a good agreement was found between the two, which supports the previous argument that the confinement is also responsible for the change in the electron g-factors. For the much less sensitive hole the same agreement was not found, indicating that the strain-dependence is governed by the effective mass instead.
with the results presented here.
Chapter 5

Active tuning of the g-tensor in InGaAs/GaAs quantum dots

Parts of this chapter were adapted from:

5.1 Introduction

Chapter 4 presented numerical calculations of the electron and hole g-tensors and diamagnetic coefficients of a biaxially strained InGaAs/GaAs quantum dot. This chapter will give an overview of the experimental realization of this system in terms of device fabrication in Sec. 5.2 and characterization in Sec. 5.3, as well as an extensive discussion of the magnetoluminescence experiments performed on this device in Sec. 5.4. The measurements result in a determination of the strain-dependence of the electron and hole g-tensors in Sec. 5.5 and the diamagnetic coefficients in Sec. 5.6. All measurements presented in this chapter are performed at a temperature of 4 K, unless indicated otherwise.

5.2 Device fabrication

Incorporating in-situ external strain in a QD layer requires some kind of actuator. Such an actuator can for example be established by embedding QDs in a bowed airbridge structure [43], however the resulting strain is rather unpredictable and inhomogeneous. A more reliable way is to integrate the QD layer on top of a piezoelectric actuator. Piezoelectric materials produce an electric field in response to external stress, or in this case vice versa. Applying a voltage across this piezoelectric actuator results in a biaxial in-plane strain in the actuator, which is transferred to the QD layer. This method is applied in this chapter and a brief overview of the device fabrication is given here.

The QDs are grown by solid source molecular beam epitaxy (MBE) [48]. On a GaAs buffer layer first a 100-nm thick Al$_{0.75}$Ga$_{0.25}$As sacrificial layer is deposited, followed by a 150-nm thick layer of intrinsic GaAs. On top of this, the InGaAs QDs are grown, which are then capped using an indium flush technique [88] to a maximum height of 2.5 nm [89]. The resulting dots have an In concentration of 20%-40% and a radius of 10-15 nm. Finally, the QDs are capped with a 150-nm-thick layer of intrinsic GaAs. By optical lithography and subsequent deposition an etch mask with gold rectangles of size 150×200 $\mu$m$^2$ is defined. After etching down to the sacrificial layer the created membranes are released by underetching the AlGaAs layer using HF. Using a flip-chip transfer onto a gold-coated piezoelectric actuator the membranes are transferred to the piezo by gold thermocompression bonding, where the two surfaces are merged by applying simultaneously both force and heat. The used piezoelectric actuator consists of [Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$]$_{0.72}$ − [PbTiO$_3$]$_{0.28}$, also known as PMN-PT, a name which will be used for the remainder of this thesis. Further details of the growth procedure and device fabrication can be found in
Chapter 5. Active tuning of the g-tensor in InGaAs/GaAs quantum dots

Figure 5.1: a) Schematic image of the final sample structure, showing the nanomembrane containing the QDs mounted on top of the piezoelectric actuator. b) Characteristic IV-curve obtained during the poling procedure. The peak between 0 and 50 V indicates the moment the dipoles align to the applied electric field.

Ref. [48]. Using a similar device, Trotta et al. [49] were able to vary the in-plane strain \( \epsilon_{||} \) by as much as \( \Delta \epsilon_{||} = \pm 0.2\% \), yielding shifts in the QD emission energy of around 15 meV.

A schematic image of the final sample structure is shown in Fig. 5.1a. Note that due to the flip-chip procedure the QDs are actually mounted upside down onto the piezoelectric actuator, i.e. the ground planes of the QDs are facing upward. As a consequence, application of a positive, out-of-plane magnetic field results in a magnetic field anti-parallel to the QD growth direction.

5.2.1 Poling procedure

On a microscopic level, the electric dipoles in the piezoelectric material are randomly oriented. Application of an electric field across the macroscopic actuator then leads to a net zero deformation. In order to activate the piezoelectric actuator and use it in the desired way, all electric dipoles need to be aligned to one another. This can simply be achieved by subjecting the device to a poling procedure, where an external electric field is applied across the piezoelectric actuator. For the piezoelectric actuators used throughout this thesis, a voltage of 200 V suffices. To prevent the device from suddenly being exposed to high levels of stress, the voltage is always slowly ramped up in steps of 2 V every 0.5 seconds. After ramping up to 200 V, the voltage is ramped back down to 0 V. This procedure aligns all microscopic electric dipoles, which can be verified by tracking the IV-
Chapter 5. Active tuning of the g-tensor in InGaAs/GaAs quantum dots

Figure 5.2: PL spectrum of a single QD for various voltages applied to the piezoelectric actuator. A linear blue shift of all lines is observed.

curve during the procedure, such as is shown in Fig. 5.1b. The IV-curve shows a hysteresis loop with a peak between 0 and 50 V which indicates the moment when the electric dipoles align. This provides an easy way to verify the functionality of the device at room temperature.

Directly after poling the device is cooled down to cryogenic temperatures, which freezes the electric dipoles and therefore preserves the piezoelectricity. In this case the bottom of the piezoelectric actuator is grounded while a voltage is applied to the top, and the device is poled in such a way that application of a positive voltage at cryogenic temperatures results in an in-plane biaxial compressive strain. In Ch. 7 the device is poled in the opposite direction to obtain a tensile strain instead.

5.3 Device characterization

The use of the diffraction limited confocal microscope described in Sec. 3.3 combined with the low QD density in the MBE-grown sample ($\leq 10^6$ cm$^{-2}$) ensures at most one QD is illuminated. This allows the measurement of photoluminescence from single quantum dots. The PL is then recorded at a temperature of 4 K while varying the voltage applied to the piezoelectric actuator. The maximum voltage applied to the piezoelectric actuator is limited to 600 V to prevent a potential breakdown in the system.

A typical PL spectrum of a single QD as a function of the voltage applied to
the piezo is shown in Fig. 5.2. Most dots that are encountered on the device emit around 1.38 eV, in good agreement with the emission energy of 1.37 eV which was calculated in the previous chapter. The different lines originate from different excitonic complexes. No fine structure splitting is observed in any of the lines within the spectral resolution (<30 µeV), as is expected for QDs with a cylinder symmetry [67]. All lines exhibit the same linear blue shift when applying stress to the system up to 1.3 meV for the maximum applied voltage of 600 V. The amount of strain transferred from the piezoelectric actuator to the QD-containing nanomembrane depends strongly on the quality of the bond between the two. For this reason the energy shift observed here is much lower than in other work using a similar device [48, 49], where energy shifts up to 15 meV were reported. Comparison with this other work yields a maximum induced strain of $\Delta \epsilon_\parallel = -0.03 \%$. Comparison with the calculations presented in Ch. 4 yields a strain of $\Delta \epsilon_\parallel = -0.028 \%$ for a shift of the emission energy of 1.3 meV. This latter value is used as a calibration for the measurements presented here, and is also indicated in Fig. 5.2.

In previous work [90] no significant differences between the different excitonic complexes were found in terms of the strain-dependence of both the emission energy and the g-factor. Therefore assignment of the specific complexes to the different spectral lines is irrelevant and it suffices to analyze only one of the lines.

### 5.4 Magneto-optical measurements

The goal of this chapter is to determine the full g-tensor for both the electron and the hole. In order to do this, the setup described in Sec. 3.3 is used. All experiments are performed at a temperature of 4 K, while the dots are excited using a 635 nm laser. Determination of the full g-tensor for the electron and hole separately requires the experiment to be executed in three different geometries; with the magnetic field parallel to the QD growth direction (Faraday geometry), perpendicular to the QD growth direction (Voigt geometry) and at an intermediate angle (here 45°). These different geometries are established by mounting the device under different angles in the cryostat and rotating the objective accordingly.

The low QD density in the nanomembranes makes it possible to retrieve the same QD in the different measurement geometries. The unique PL spectrum of each QD is then used to verify that the same QD is indeed being observed. With this approach in total five different QDs have been studied individually. Any results shown in the figures in the following correspond to the same QD as the spectra shown in Fig. 5.2 were obtained from. Later results obtained from other
the QDs are tabulated in order to show the consistency of the observations.

The PL spectrum of a single QD upon exposure to external fields up to 8 T in the three different geometries is shown in Fig. 5.3. The insets show the orientation of the magnetic field. Both the Zeeman splitting and the diamagnetic shift are clearly visible. In the Faraday geometry only two of the four states are optically active (bright states) due to the conservation of spin, whereas the other two states are not optically active (dark states) as was already explained in Sec. 2.6. Indeed the single line at zero magnetic field is observed to split up into two peaks at non-zero magnetic fields. In the other two geometries, mixing of the bright and dark states causes all four lines to become visible at non-zero magnetic fields. Note that in the Voigt geometry an additional complex comes up at higher magnetic fields. Because of this additional complex, for this particular dot the lines belonging to the complex under investigation can only be accurately distinguished at magnetic
fields up to 8 T, as at higher magnetic field strengths the two complexes begin to overlap.

Since no fine structure splitting is observed at zero magnetic field and the splitting of the lines at non-zero magnetic fields is completely symmetrical, the exchange interaction can be fully disregarded. Eq. 2.43 can be applied to the three different geometries. In the Faraday geometry the splitting between the two lines is characterized by the exciton g-factor $g_F$ which is defined by the sum of the out-of-plane hole and electron g-factors, $g_{h,z} + g_{e,z}$. In the Voigt geometry, the splitting of the four lines is characterized by two g-factors $g_{V1}$ (difference between the outer two peaks) and $g_{V2}$ (difference between the inner two peaks) which are determined by the sum and the difference between the in-plane hole and electron g-factors, however it is not known which set of peaks corresponds to which combination of electron and hole g-factors. Finally the splitting of the four lines in the intermediate geometry is characterized by two g-factors $g_{I1}$ (outer peaks) and $g_{I2}$ (inner peaks) which are combinations of the in-plane and out-of-plane electron and hole g-factors. In this case the outer two peaks can be explicitly assigned to a combination of electron and hole g-factors, while only the ordering of the inner two peaks is unknown, as it is determined by the relative magnitude of the hole g-factors compared to the electron g-factors. The measured values of the g-factors have to satisfy the set of equations

$$
\begin{align*}
g_F &= g_{h,z} + g_{e,z}, \\
g_{V1} &= g_{h,x} \pm g_{e,x}, \\
g_{V2} &= g_{h,x} \mp g_{e,x}, \\
g_{I1} &= \frac{1}{\sqrt{2}} \left( \sqrt{g_{e,x}^2 + g_{e,z}^2} + \sqrt{g_{h,x}^2 + g_{h,z}^2} \right), \\
g_{I2} &= \frac{1}{\sqrt{2}} \left( \sqrt{g_{e,x}^2 + g_{e,z}^2} - \sqrt{g_{h,x}^2 + g_{h,z}^2} \right). 
\end{align*}
$$

Since the signs of the measured quantities are not known, solving this system leads to the absolute values of the in-plane and out-of-plane electron and hole g-factors, given by $|g_{h,z}| = 1.56 \pm 0.01$, $|g_{h,x}| = 0.14 \pm 0.01$, $|g_{e,z}| = 0.46 \pm 0.01$ and $|g_{e,x}| = 0.4 \pm 0.01$.

**Sign assignment**

Some extra analysis is required to determine the signs of the g-factors. Analogous to Ch. 4, the sign is defined in such a way that when a magnetic field is applied along a certain axis and the state with a negative total-momentum projection onto this axis is the ground state, the g-factor is considered to be positive [86].
For the out-of-plane g-factors this analysis is relatively straightforward. From the splitting of the two peaks the absolute value of the exciton g-factor can be determined. The two visible transitions emit right-handed circularly polarized light (\(\sigma^+\)) and left-handed circularly polarized light (\(\sigma^-\)). The Zeeman splitting between the two peaks is given by

\[
\Delta E_{\text{Zeeman}} = E(\sigma^+) - E(\sigma^-) = \mu_B B_0 g_F.
\]

By determining the polarization of the peaks, the sign of the exciton g-factor can be determined from which the signs of the out-of-plane electron and hole g-factors immediately follow.

The polarization is determined by inserting a \(\lambda/4\)-plate and a linear polarizer into the collection arm. The \(\lambda/4\)-plate transforms the circular polarization of the emission into linear polarization [91]. The polarizer then selects the desired polarization.

By changing the orientation of the polarizer with respect to the \(\lambda/4\)-plate, the ratio between the intensities of the two peaks, \(I_1\) and \(I_2\), of the Zeeman split doublet is affected. It should be noted that also the total intensity of the two peaks combined, \(I_1 + I_2\), changes since physically rotating either the polarizer or the \(\lambda/4\)-plate affects the alignment of the system. In this case the \(\lambda/4\)-plate is rotated since it is equivalent to rotating the polarizer and the alignment was found to be less affected than when rotating the polarizer itself. The peak intensities \(I_1\)
and $I_2$ are normalized to the total intensity $I_1 + I_2$ to obtain the relative peak intensities, which are plotted in Fig. 5.4 for different orientations of the $\lambda/4$-plate. When the degree of circular polarization is 100%, the relative intensities of the two peaks should be given by $\sin^2 x$ and $\cos^2 x$ respectively. Both are indicated in Fig. 5.4 and agree well with the experimental data. By carefully considering the initial orientation of the polarizer with respect to the $\lambda/4$-plate and the orientation of the magnetic field with respect to the QD growth axis, the sign of the exciton g-factor is determined to be negative. As a consequence, both the out-of-plane electron and hole g-factors are negative as well. For the in-plane components the situation is more complicated. In the Voigt geometry, an external magnetic field leads to linear polarization. The two different linear polarizations can be distinguished, but not unambiguously assigned to either of the peaks. The sign can therefore not be determined this way. Instead the sign of the in-plane g-factors is deduced from the fact that is known from both the numerical calculations presented in Ch. 4 and other reported experiments [19, 28, 92] that generally the electron g-factor increases with increasing emission energy. By comparing this with the strain-dependence of the electron g-factors which will be presented in Sec. 5.5 it is concluded that the sign the in-plane electron g-factor is negative. The sign of the in-plane hole g-factor is inferred from the numerical calculations presented in Sec. 4 and is negative.

### 5.5 Strain-dependence of the g-tensors

By repeating the measurement described in Fig. 5.3 while varying the voltage applied to the piezoelectric actuator, the strain-dependence of the g-factors can be obtained. The result is shown in Fig. 5.5, where the out-of-plane and in-plane electron and hole g-factors are plotted as function of the voltage applied to the piezoelectric actuator.

The g-tensor for the hole shows a remarkable anisotropy; the out-of-plane hole g-factor exhibits a relatively large shift, whereas the in-plane value is virtually unaffected. As the amount of strain varies from membrane to membrane and the shift in emission energy scales linearly with the induced strain, the sensitivities of the g-tensor components (i.e. the slopes of the lines in Fig. 5.5) are given in terms of the shift in emission energy. This also allows for an easier comparison with the calculations presented in Ch. 4. The slopes are $dg_{h,z}/dE = 0.051 \text{ meV}^{-1}$ and $dg_{h,x}/dE = 0.001 \text{ meV}^{-1}$. The opposite anisotropy occurs for the electron, however less pronounced. The electron g-factor shows only a limited change in both directions, with slopes of $dg_{e,z}/dE = -0.001 \text{ meV}^{-1}$ and $dg_{e,x}/dE = 0.005 \text{ meV}^{-1}$. 


Figure 5.5: Experimentally determined value for the electron (black) and hole (red) g-factors, both a) out-of-plane and b) in-plane as a function of voltage applied to the piezoelectric actuator. The values are obtained by combining results for the Zeeman splitting in three different geometries, applying magnetic fields up to 10 T. Shaded areas indicate the error range.

Table 5.1: Emission energy, g-factors and their sensitivities for five different dots, showing the consistency of the results. Sensitivities for the g-factors are given in change per eV of shift in emission energy.

<table>
<thead>
<tr>
<th>Dot</th>
<th>E</th>
<th>$g_{h,z}$</th>
<th>$g_{h,x}$</th>
<th>$g_{e,z}$</th>
<th>$g_{e,x}$</th>
<th>$\frac{dg_{h,z}}{dE}$</th>
<th>$\frac{dg_{h,x}}{dE}$</th>
<th>$\frac{dg_{e,z}}{dE}$</th>
<th>$\frac{dg_{e,x}}{dE}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.383</td>
<td>-1.56</td>
<td>-0.14</td>
<td>-0.46</td>
<td>-0.40</td>
<td>51</td>
<td>1</td>
<td>-1</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>1.383</td>
<td>-1.86</td>
<td>-0.32</td>
<td>-0.41</td>
<td>-0.31</td>
<td>37</td>
<td>4</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>1.380</td>
<td>-2.35</td>
<td>-0.27</td>
<td>-0.40</td>
<td>-0.54</td>
<td>49</td>
<td>8</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>1.385</td>
<td>-1.71</td>
<td>-0.21</td>
<td>-0.43</td>
<td>-0.41</td>
<td>41</td>
<td>7</td>
<td>-1</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>1.377</td>
<td>-1.74</td>
<td>-0.16</td>
<td>-0.52</td>
<td>-0.31</td>
<td>40</td>
<td>-8</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>Avg.</td>
<td>1.382</td>
<td>-1.84</td>
<td>-0.22</td>
<td>-0.45</td>
<td>-0.39</td>
<td>43</td>
<td>2</td>
<td>1</td>
<td>5</td>
</tr>
</tbody>
</table>

To investigate the consistency of this result, in total five different single QDs are studied. The emission energies, g-factors and their slopes of all investigated dots are listed in Table 5.1. Due to the limited spread in the absolute values of the g-factors, the sign assignment for the QD in Fig. 5.5 is also valid for the rest of the dots. In general the agreement between the different dots in terms of g-factors and their sensitivities is excellent.

Finally the experimentally determined g-factors and their sensitivities are compared to the ones that followed from the numerical calculations in Table 5.2. The experimental results are very well reproduced by the calculations in terms of the
sensitivities for all components. The physical origins of the changes in the different
g-factors illustrated in Ch. 4 are therefore validated.

It should be noted that there are some discrepancies between the calculations
and experiments in the absolute values of the g-factors. The geometries used
in the calculations are an estimate for the real dots, but are probably not 100%
accurate. By exploring the parameter space around this typical dot, the calculated
g-factors can be tuned closer to the experimental values. However, when varying
the dot height from 1.5 to 5 nm, the dot radius from 5 to 15 nm and the Indium
concentration from 30 to 50%, no significant changes (<10%) in the sensitivities
of the different components were observed. Therefore the dot parameters were
not optimized in Ch. 4, since the observed sensitivities are quite robust against
a variation of them. The different components of the electron and hole g-tensors
will now be addressed one by one.

\( g_{h,z} \): The nominal values of \( g_{h,z} \) range from -2.4 to -1.6. This relatively wide
variation is not unusual, as the hole g-factor is known to be extremely sensitive
to the exact size, shape, composition and built-in strain of the QD \cite{25, 28}. The
out-of-plane hole g-factor shows by far the largest sensitivity to the applied strain,
with the slope ten times larger than any of the other components. The result is
consistent for all dots, with slopes ranging roughly from 0.04-0.05 meV\(^{-1}\). The
observed shift is remarkably large considering the limited amount of strain deliv-
ered to the QD and agrees well with the numerical calculations where a sensitivity
of 0.051 meV\(^{-1}\) was found. In the calculations it was found that the change in
the out-of-plane hole g-factor is mainly caused by a change in the heavy hole-light
hole mixing in the hole ground state.

\( g_{h,x} \): The in-plane hole g-factor shows much smaller nominal values, ranging from
-0.15 to -0.3. The sensitivity to strain is therefore also smaller, however the slopes
show a rather large spread, even changing sign for one of the dots. This agrees
well with the numerical calculations, where an in-plane hole g-factor of -0.1 was
found with negligible sensitivity to strain. This anisotropy between the in-plane
and out-of-plane hole g-factor is well-known for a heavy hole \cite{67}, which is the
dominating character in the ground state hole wavefunction due to the symmetry
of the dot.

\( g_{e,z} \): The nominal value of \( g_{e,z} \) shows only a small spread, with all values being
around -0.45. For most dots, the out-of-plane electron g-factor shows no signific-
ant sensitivity to strain. Averaging over all dots a negligible increase in \( g_{e,z} \)
of 0.001 meV\(^{-1}\) is found. The same small increase was found in the numerical
### Table 5.2: Values of the g-factors and their sensitivities to strain determined from both the numerical calculations and the experiment. The sensitivities $\delta g/\delta E$ show a good agreement between the two.

<table>
<thead>
<tr>
<th>Component</th>
<th>Calculation Value</th>
<th>$dg/dE$ eV$^{-1}$</th>
<th>Experiment Value</th>
<th>$dg/dE$ eV$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{h,z}$</td>
<td>-2.584</td>
<td>51</td>
<td>-1.84</td>
<td>43</td>
</tr>
<tr>
<td>$g_{h,x}$</td>
<td>-0.102</td>
<td>0</td>
<td>-0.22</td>
<td>2</td>
</tr>
<tr>
<td>$g_{e,z}$</td>
<td>-0.057</td>
<td>1</td>
<td>-0.45</td>
<td>1</td>
</tr>
<tr>
<td>$g_{e,x}$</td>
<td>0.171</td>
<td>6</td>
<td>-0.39</td>
<td>5</td>
</tr>
</tbody>
</table>

In the majority of the dots the value of $g_{e,x}$ is slightly higher than $g_{e,z}$. This small anisotropy is known from experiments [17, 25] and was also found in the numerical calculations and explained by considering the orbital momentum quenching which is stronger in the growth direction of the dot. The in-plane electron g-factor shows the same sensitivity to strain in all dots, with a shift of 0.005 meV$^{-1}$, which is in excellent agreement with the 0.006 meV$^{-1}$ found in the calculations and caused by a decrease of the lateral extension of the electron wavefunction in the growth direction of the QD. Since this effect is stronger in the growth direction compared to the radial direction, the sensitivity of $g_{e,x}$ is larger compared to $g_{e,z}$.

#### 5.6 Diamagnetic shift

To further emphasize the effect of strain on the lateral extension of the electron wavefunction in both radial and the growth direction of the QD, the strain-dependence of the exciton diamagnetic coefficient $\alpha_d$ is investigated as it is a direct probe of the size of the electron wavefunction. As was shown by the calculations in Sec. 4.7, the contribution of the hole to the exciton diamagnetic coefficient can be neglected since it scales with the inverse effective mass.

The diamagnetic coefficient in the Faraday geometry is obtained by fitting the average position of the Zeeman split doublet (or quadruplet in the Voigt geometry) as a function of magnetic field with a quadratic dependence. This is done for one QD for different amounts of induced strain by varying the voltage applied to the piezoelectric actuator, the result of which is shown in Fig. 5.6a. The
Figure 5.6: a) In-plane and out-of-plane diamagnetic coefficients of a single QD as a function of the voltage applied to the piezoelectric actuator. Both decrease with increasing strain, indicating a decrease in the lateral extension of the electron wavefunction. b) Calculated exciton diamagnetic coefficients (from Ch. 4) showing the same trends as the experiment.

other four QDs show the same trends. The diamagnetic coefficients in the Faraday and Voigt geometries are 12 and 4 \( \mu eV/T^2 \) respectively in the absence of induced strain. This agrees well with the combined diamagnetic coefficients \( \alpha_{d}^e + \alpha_{d}^h \) obtained from the numerical calculations in Fig. 5.6b, which have values of 9.2 and 4.3 \( \mu eV/T^2 \) for magnetic fields applied out-of-plane and in-plane respectively. The small discrepancy between the calculated and experimentally determined out-of-plane diamagnetic coefficient can be accounted for by an underestimation of the QD radius in the calculations.

The circulating currents related to the diamagnetic coefficient are perpendicular to the direction of the magnetic field. As a result, when applying the magnetic field parallel to the QD growth direction the lateral extension in the plane of the QD is relevant, and vice versa. The anisotropy of the diamagnetic coefficient, which is larger in the Faraday geometry compared to the Voigt geometry can therefore easily be explained from the high aspect ratio of the QDs.

When inducing biaxial compressive strain in the QD, for both geometries the diamagnetic coefficient decreases. This proves that indeed the lateral extension of the electron wavefunction decreases in all directions due to an increase of the confinement energy. This anisotropy was also observed in the calculations and is caused by the fact that the leakage of the electron wavefunction into the surrounding GaAs barrier is much more pronounced in the QD growth direction.

The influence of induced strain on the diamagnetic coefficients is remarkable, changing 5 % and 1 % for the Voigt and Faraday geometries respectively, even though the strain is only changed by \( \Delta \varepsilon || = -0.03 \% \). The large sensitivity can be
understood when realizing that the electron is only weakly confined to the QD and a small change in the strain environment has a relatively large effect on the confinement energy of the electron, leading to a large impact on the lateral extension of the electron wavefunction. In the numerical calculations comparable changes of 4.1 % and 1.4 % at a three times larger strain of $\Delta \epsilon_{\parallel} = -0.1 \%$ were obtained, leading to the conclusion that even though the calculations predict the correct trend for the strain-dependence of the diamagnetic coefficients, the magnitude of the sensitivity is even larger than the calculations predict. This could possibly be explained by an overestimation of the confinement energy in the calculations. If the confinement energy is even smaller than the $\approx 25 \text{ meV}$ that was found in the calculations, for example due to a slightly larger In-concentration or smaller QD height, the electron wavefunction would be less localized and the effect of strain would be larger.

Using the electron effective mass for In$_{0.4}$Ga$_{0.4}$As $m_e = 0.048 \ m_0$, which is calculated using the parameters from Ref. [80], and Eq. 4.4, the lateral extension of the electron wavefunction can be calculated from the diamagnetic coefficients. In the Faraday geometry this leads to $l_{x,y} = 5.12 \ \text{nm}$, which decreases to 5.09 nm at $\Delta \epsilon_{\parallel} = -0.03 \%$. In the Voigt geometry the lateral extension is $l_{y,z} = 2.93 \ \text{nm}$, which decreases to 2.84 nm at $\Delta \epsilon_{\parallel} = -0.03 \%$. This means that in these measurements the diamagnetic shift can be used to probe changes in the lateral extension of the electron wavefunction with sub-angstrom precision.

### 5.7 Conclusions

The strain-dependence of the full g-tensor for both the electron and hole has been experimentally investigated using a piezoelectric actuator to apply biaxial compressive strain to QDs integrated on top of it. A remarkable sensitivity of the out-of-plane hole g-factor $g_{h,z}$ has been found. The in-plane electron g-factor $g_{e,x}$ showed moderate sensitivity, while the sensitivities of the other two components $g_{h,x}$ and $g_{e,z}$ are barely detectable within the accuracy of the experiment. This result is consistent in all five investigated QDs and the behavior of all components agrees well with the $k \cdot p$-calculations presented in Ch. 4.

The electron g-tensor was found to show a small increase with applied strain for both components. Anisotropy between the two different components was observed. Both were explained by considering the change in orbital momentum quenching due to the leaking of the wave function into the surrounding barrier. This was experimentally verified by determining the diamagnetic coefficient as a function of induced strain, where it was found to decrease in both the Faraday
and Voigt geometries, indicating a decrease in the lateral extension of the electron wavefunction in all directions.

The hole g-tensor showed a similar anisotropy in both nominal value and sensitivity, with the large out-of-plane g-factor experiencing a large change and the small in-plane g-factor experiencing a small change. Since this compares well with the numerical calculations presented in the previous chapter, the same conclusion can be drawn; the large sensitivity of the out-of-plane hole g-factor is related to the strong HH-like character of the hole ground state and the change of the LH contribution with induced strain.

As stated in the introduction of this thesis, tunability of one of the g-tensor components around zero would be technologically most relevant [31]. For this purpose, the out-of-plane hole g-factor is the most suitable candidate. By size engineering of the QDs, the nominal value of the g-factor can be brought close to zero, in absence of external strain. Additionally, a much larger tuning range can be achieved by making use of more advanced devices [93, 94, 95] with reported strain values up to 1.5 % [96]. In some of these devices, full anisotropic control of over the in-plane strain tensor is possible. This opens up a new way of manipulating the g-tensor per component, both in the conduction and valence band.
Chapter 5. Active tuning of the g-tensor in InGaAs/GaAs quantum dots
Chapter 6

Strain and g-tensors in an InAsP nanowire quantum dot

To be published.
6.1 Introduction

The previous two chapters have extensively discussed the strain-dependence of the electron and hole g-tensors in self-assembled quantum dots which were grown in the ZB crystal structure. In Ch. 4 a numerical model based on \( k \cdot p \) theory was successfully employed to support the experiments in Ch. 5. The model was able to explain the experimental results both qualitatively and quantitatively, therefore granting valuable insight in the underlying physical mechanisms.

In Ch. 7 magneto-luminescence experiments are reported on WZ InAsP nanowire quantum dots (NWQDs). By determining the Zeeman splitting for various orientations of the magnetic field with respect to the NWQD growth axis, the electron and hole g-tensors are determined. By means of a piezoelectric actuator, uniaxial stress along the growth direction is exerted on the NWQDs to investigate the strain-dependence of the g-tensors. The aim of the current chapter is to support these experiments and predict the strain-dependence of the electron and hole g-tensors.

For most ZB III-V semiconductors all parameters required to perform full \( k \cdot p \) calculations have been well known for years. For WZ InAs and InP many of these parameters are not yet known. A simplified model, which makes use only of known parameters such as band edge energies and effective masses, is therefore highly desirable. The aim of this chapter is to develop a primitive model for the calculation of the electron and hole g-factors in WZ nanostructures. In a WZ system the behavior of electron and hole states when they are exposed to an external magnetic field is expected to be fundamentally different due to the different symmetry of the crystal structure. While ZB materials require an asymmetric confining potential to obtain anisotropy in the electron g-tensor, this anisotropy is already present in bulk WZ due to the hexagonal crystal structure. This anisotropy has for example been observed in hexagonal AlGaN [97] where \( g_z > g_x \). Magneto-optical experiments on other bulk WZ III-V’s have so far mainly focused on InP, however the electron and hole g-tensors have not been fully disentangled. De Luca et al. [98] have reported an in-plane electron g-factor of \( g_{e,x} = 1.4 \) by assuming the in-plane hole g-factor to be negligible and an out-of-plane exciton g-factor \( |g_{e,z} - g_{h,z}| = 3.5 \). Similar values of \( g_{e,x} = 1.29 \) and \( |g_{e,z} - g_{h,z}| = 4.66 \) have been reported by Tedeschi et al. [99]. For GaAs WZ nanowires a value of \( g_{e,x} \approx 0 \) was reported [100]. Comparing these experimentally known values for InP and GaAs with their ZB counterparts (GaAs: \( g_e = -0.44 \), InP: \( g_e = 1.26 \)) indicates a trend where \( g_{WZ} > g_{ZB} \). This trend has also been observed for GaN [97].

An analytical expression for the electron g-factors in WZ analogous to the Roth formula in ZB was derived by Hermann and Weisbuch [101]. They tacitly
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

assumed the optical matrix element to be isotropic, which is not entirely valid due to the anisotropic crystal structure of WZ. Besides the bottom conduction band and top three valence bands, their approach also includes higher conduction bands. These higher conduction bands are relevant for wide-gap materials such as GaN [102], but do not have to be taken into account for most other III-V’s due to the smaller band gap relative to the separation between the conduction band levels. This simplification has been used by Faria Junior et al. [103] to calculate the g-factors for bulk WZ InP. Their approach yields a good agreement with the available experimental data, but has not yet been applied to nanostructures.

For the calculation of the valence band g-factor it is required to take the coupling between the different valence bands carefully into account. An approach to do this for bulk WZ materials was presented by Rodina et al. [104] and successfully applied to GaN. Their approach can be extended to InAs and InP to estimate the strain-dependence of the hole g-factors in an InAsP NWQD.

In this chapter the work of Faria Junior et al. and Rodina et al. is extended with strain and quantization energy calculations to investigate the strain-dependence of the electron and hole g-tensors in a WZ nanostructure. The chapter is organized as follows. An overview of the required parameters and how they are obtained is given in Sec. 6.2. The strain distribution in an InAsP NWQD is calculated using a finite element method in Sec. 6.3. The band edge energies in the NWQD and their strain-dependence are calculated using these strain distributions in Sec. 6.4.

A common approach to evaluate the electron g-factor in nanostructures is to use an adapted Roth formula, where the band gaps in the standard expression are modified to include the additional confinement energies occurring in QDs [25, 34, 105]. Quantization energies are calculated in Sec. 6.5 using a one-band effective mass model. In Sec. 6.6 the formalism underlying the Roth formula is applied to the basis Bloch functions of WZ materials to obtain an analytical expression for the electron g-factors for WZ, analogous to the work of Hermann and Weisbuch [101] but with anisotropic momentum matrix elements. The strain-dependence of the electron g-tensor is calculated in Sec. 6.7. The strain-dependence of the hole g-tensor is then estimated in Sec. 6.8 followed by some concluding remarks in Sec. 6.9.
6.2 Wurtzite parameters for InAs and InP

The NWQDs in Ch. 7 consist of a section of InAsP encapsulated in an InP nanowire. In order to calculate the strain-dependence of the g-factors, a number of material parameters for WZ InAs, InP and InAsP is required. To perform the strain calculations, only the lattice constants and elastic constants need to be known. The electronic calculations require many parameters; band edge energies, band offsets, effective masses and deformation potentials. In most cases these parameters are known experimentally, while for the remaining parameters theoretical estimates are available. Parameters for the InAsP alloy are obtained via linear interpolation between InAs and InP, unless stated otherwise.

Lattice constants

The lattice constants for WZ, assuming a non-distorted lattice, are derived from the ZB lattice constant $a_{ZB}$ via $a_{WZ} = \sqrt{\frac{1}{2}} a_{ZB}$ and $c_{WZ} = \sqrt{\frac{4}{3}} a_{ZB}$. Experimentally known lattice constants meet this non-distorted approximation very well, as was previously shown in Table 2.1.

Elastic constants

In Ch. 2 elastic constants ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, $C_{44}$ and $C_{66}$) for WZ materials were obtained via a transformation from their ZB counterparts. The resulting values were compared with results from DFT calculations and a good agreement was found (see Table 2.2). Therefore the elastic constants resulting from the DFT calculations will be used here.

InP band edges

In literature the three valence bands are often labelled A (heavy hole), B (light hole) and C (crystal field split hole). This notation will also be used here. The band structure of WZ at the Γ-point is depicted in Fig. 6.6a and is characterized by a band gap, $E_g = E_A$, and two splittings in the valence band, $E_{AB}$ and $E_{AC}$. For WZ InP the band edge energies are extensively reported in literature. The most common value for the band gap itself is 1.49 eV, while the valence band splittings (i.e. the difference between the HH band and the LH and CH bands) are reported to lie in the range of $E_{AB} = 30 - 50$ meV and $E_{AC} = 140 - 200$ meV according to both theoretical [51, 106, 107, 108, 109, 110] and experimental [110, 111, 112, 113, 114, 115] studies. Values of 40 meV and 170 meV will therefore be used here, corresponding to a crystal field splitting of $\Delta_{cf} = 76$ meV and a spin-orbit splitting of $\Delta_{so} = 134$ meV.
### Table 6.1: Parameters for WZ InAs, InP and InAs$_{0.3}$P$_{0.7}$

Sources of the parameters are discussed in the text.
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

InAs band edges

For WZ InAs the band gap is experimentally determined to be 0.48 eV \[116, 117, 118\] which agrees well with theoretical studies \[51, 106, 119\]. As of yet, the valence band splittings have not been determined experimentally but are given by various theoretical estimates in the range of \(E_{AB} = 60 - 70\) meV and \(E_{AC} = 350 - 360\) meV \[119, 120, 107\], corresponding with \(\Delta_{cf} = 101\) meV and \(\Delta_{so} = 339\) meV.

InAsP band edges

The band edge energies of the InAsP alloy are obtained by interpolating the crystal field and spin-orbit splittings and calculating the band edge energies using Eq. 2.31. Note that due the non-linear dependence of the band edge energies on \(\Delta_{so}\) and \(\Delta_{cr}\) this is not equivalent to interpolating the band edges of InAs and InP directly, however the difference is negligible (< 5 meV).

Band offsets

In order to calculate the quantization energy in the different bands it is crucial to know the band offsets between InAs and InP. In Ref. \[51\], De & Pryor give band offsets between WZ materials and their ZB counterparts. Using the ZB offsets known from Ref. \[80\] the valence band offset (VBO) between WZ InAs and InP can be calculated to be 240 meV. DFT calculations performed by Hajlaoui et al. \[121\] yield a conduction band offset (CBO) of 560-680 meV and a VBO of 330-380 meV. Persson at al. \[122\] have experimentally determined the CBO to be 740 meV from electrical transport measurements performed on InAs nanowires containing a segment of InP, leading to a VBO of 270 meV. The latter will be used since it is the only available experimental value and is in good agreement with the theoretical estimates.

Effective masses

In bulk WZ the effective mass is anisotropic and each band has an effective mass \(m^{\parallel}\) parallel to the c-axis and \(m^{\perp}\) perpendicular to the c-axis. Effective masses have been calculated by De & Pryor using pseudopotentials \[51\] and by Faria Junior et al. using a multiband \(k \cdot p\)-model \[107\]. The agreement between the two sets is good, the main difference lying in the anisotropy of the effective mass in the bottom conduction band, where \(m^{\parallel} > m^{\perp}\) according to Ref. \[51\] and \(m^{\parallel} < m^{\perp}\) according to Ref. \[107\]. The latter has been experimentally demonstrated for WZ InP \[123, 124\] as well as for other non-III-V WZ materials such as GaN \[125\]. Therefore the effective masses from Ref. \[107\] will be used here.
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

Deformation potentials

For ZB materials the strain-dependence of the band edges is defined by four deformation potentials; $a_c$ for the conduction band and $a_v$, $b$ and $d$ for the valence bands. For the WZ crystal structure this is extended to six deformation potentials on which the band edge energies depend according to Eq. 2.32; $a_{cz}$ and $a_{ct}$ for the conduction band and $D_1$, $D_2$, $D_3$ and $D_4$ for the valence band. Hajlaoui et al. [126] have performed DFT calculations to obtain the deformation potentials of WZ InAs and InP. Their calculated values agree well with a pressure-dependent PL study on InP nanowires performed by Chauvin et al. [127]. The disadvantage of the set of deformation potentials given by Hajlaoui et al. is that they are related to the band gap rather than the conduction and valence band separately.

In the quasi-cubic approximation, where the WZ structure is considered as a ZB structure strained along the [111]-direction, the WZ deformation potentials can be directly derived from the ZB ones [128]. The conduction band is then unchanged from ZB and $a_{cz} = a_{ct} = a_c$ [129], while the deformation potentials for the valence band are given by

\[
D_1 = a_v + \frac{2d}{\sqrt{3}} \quad D_2 = a_v - \frac{d}{\sqrt{3}} \\
D_3 = -\sqrt{3}d \quad D_4 = \frac{3d}{2\sqrt{3}}.
\] (6.1)

Deformation potentials calculated by Hajlaoui et al. and obtained via the quasi-cubic (QC) approximation are given in Table 6.2. For some deformation potentials the agreement is good, but for others the agreement is quite poor. Since the theoretical results from Hajlaoui et al. are able to reproduce the experimental results from Ref. [127], these values are deemed more reliable. To account for the fact that only $a_{cz} - D_1$ and $a_{ct} - D_2$ are known rather than the deformation potentials for the conduction and valence bands separately, the quasi-cubic approximation is applied to the conduction band (i.e. $a_{cz} = a_{ct} = a_c$). This is then combined with the DFT results from Ref. [126] to obtain the complete set of deformation potentials.

<table>
<thead>
<tr>
<th>Mat</th>
<th>Source</th>
<th>$a_c$</th>
<th>$D_1$</th>
<th>$D_2$</th>
<th>$D_3$</th>
<th>$D_4$</th>
<th>$a_{cz} - D_1$</th>
<th>$a_{ct} - D_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>InAs</td>
<td>QC</td>
<td>-5.08</td>
<td>-5.16</td>
<td>1.08</td>
<td>6.24</td>
<td>-3.12</td>
<td>0.08</td>
<td>-6.16</td>
</tr>
<tr>
<td>InAs</td>
<td>Ref. [126]</td>
<td>-5.85</td>
<td>-3.17</td>
<td>-2.69</td>
<td>-8.33</td>
<td>0.01</td>
<td>-7.92</td>
<td></td>
</tr>
<tr>
<td>InP</td>
<td>QC</td>
<td>-6.00</td>
<td>-6.01</td>
<td>1.92</td>
<td>7.93</td>
<td>-3.97</td>
<td>0.01</td>
<td>-7.92</td>
</tr>
<tr>
<td>InP</td>
<td>Ref. [126]</td>
<td>5.92</td>
<td>-3.28</td>
<td>5.92</td>
<td>-3.28</td>
<td>5.92</td>
<td>-3.28</td>
<td></td>
</tr>
</tbody>
</table>

*Table 6.2: Deformation potentials of InAs and InP derived from the quasi-cubic approximation (QC) and obtained from Ref. [126].*
Strain and g-tensors in an InAsP nanowire quantum dot

potentials listed in Table 6.1, where an overview is given of all relevant parameters for WZ InAs, InP and InAs$_{0.3}$P$_{0.7}$.

### 6.3 Strain calculations

In order to calculate the strain-dependence of the g-tensor, the strain profile in the QD and its response to external stress is required. In Ch. 4 this was realized by applying continuum elasticity theory to a real space grid onto which the nanostructure was projected. External stress was mimicked by introducing a stressor layer below the QD structure, resulting in biaxial strain. In this case such an approach is not feasible, since the stress needs to be applied uniaxially along the c-axis of the WZ crystal structure. The strain calculations presented here are performed using Comsol Multiphysics where external forces can be incorporated directly to achieve the desired stress configuration.

The first step is to obtain the built-in strain profile caused by the lattice mismatch between the InAsP dot and the InP host. Since Comsol uses continuum mechanics, the lattice mismatch between the different materials, which takes place on the atomic level, cannot be implemented directly. Instead, the lattice mismatch is mimicked by introducing an initial strain $\epsilon_{IS}$ in the QD material equal to

$$\epsilon_{IS} = \frac{a_{QD} - a_{NW}}{a_{QD}},$$

where $a_{QD}$ and $a_{NW}$ are the lattice constants of the dot material and the wire material respectively. This results in the required elastic energy which will relax upon computation of the model. Finally, this initial strain has to be subtracted from the computed result to obtain the real, physical strain profile.

The wire, which consists of pure WZ InP, has a length $l_w$ of 300 nm, which is long enough for the strain to be relaxed at the end of the wire. The dot has a hexagonal ground plane with a radius $r_{QD}$ of 10 nm, where the radius is defined as the distance from the center of the hexagon to one of its corners. The dot has a height $h$ of 5 nm, and consists out of WZ InAs$_{0.3}$P$_{0.7}$. The structure is covered with a pure WZ InP shell with a thickness $r_s$ of 100 nm. These parameters are representative for the NWQDs discussed in Ch. 7. Additional strain can be induced by applying a force $F$ to both ends of the nanowire. Due to mirror symmetry of the structure in the $xy$-, $xz$- and $yz$-planes only one eighth of the entire structure has to be modelled. The simulated structure is schematically shown in Fig. 6.1.

Figure 6.2 shows the result of the strain calculations for the $z$-component of the strain ($\epsilon_{zz}$, top panel), the $y$-component ($\epsilon_{yy}$, middle panel) and the $x$-component
Figure 6.1: Schematic representation of the modelled structure. Only one eighth of the shown structure is actually modelled due to the symmetry in the xy-, xz- and yz-planes.

(\(\epsilon_{xx}\), bottom panel). These components are plotted on the \(xy\)-, \(xz\)- and \(yz\)-cross-sections through the center of the QD. The strain calculation results in only one quadrant of each plot, which has been duplicated in two directions for visibility.

The \(xy\)-cross-section of \(\epsilon_{zz}\) shows predictable behaviour near the edge of the QD; tensile strain in the outer, lower lattice constant, nanowire material and compressive strain in the inner, higher lattice constant, QD material. Analogous to the self-assembled QDs in Sec. 4.3, the strain changes from compressive towards tensile when moving from the edge to the center of the dot. This is caused by the Poisson effect, where the compression in the \(x\)- and \(y\)-directions leads to a net tensile strain the \(z\)-direction in the center of the dot due to the high aspect ratio of the QD. Averaged over the entire dot \(\epsilon_{zz} = -0.01\%\). Even close to the edge of the QD the strain profile does not resemble the hexagonal shape of the QD but rather exhibits a cylindrically symmetric behavior. This suggests that the QD may be approximated quite well by a cylindrical potential. The \(x\)- and \(y\)-components of the strain tensor, \(\epsilon_{xx}\) and \(\epsilon_{yy}\), are homogeneously compressive across the entire QD. Averaged over the entire dot \(\epsilon_{xx} = \epsilon_{yy} = -0.6\%\).

The most insightful way to show the effect of an external force applied to the nanowire is to plot the different components of the strain tensor for different applied pressures. This is shown in Fig. 6.3 for different lines crossing the center of the dot for highly exaggerated values of strain to emphasize the trends.

Contrary to what was found for the cylindrical symmetric system in Ch. 4, \(\epsilon_{xx}\) in the \(x\)-direction differs slightly from \(\epsilon_{yy}\) in the \(y\)-direction due to the hexagonal ground plane. In the \(z\)-direction \(\epsilon_{xx}\) and \(\epsilon_{yy}\) are identical. Applying a uniaxial stress to the wire doesn’t actually change the strain profile in the wire, it only
Figure 6.2: Diagonal components of the strain tensor plotted on the $xy$-, $xz$- and $yz$-planes through the center of the dot.
introduces an offset. The induced strain is homogeneous across the entire wire. Application of a positive force to the ends of the wire leads to an induced tensile strain in the $z$-direction which is accompanied by a smaller, compressive strain in the $x$- and $y$-directions. This is emphasized in Fig. 6.4, which shows the average of the strain-components $\epsilon_{xx}$, $\epsilon_{yy}$ and $\epsilon_{zz}$ in the QD as a function of the force applied to the wire. All three diagonal components of the strain tensor shift linearly with the applied pressure over a wide range. To check the accuracy of the strain calculations, it is worthwhile to calculate the Poisson ratio $\nu$ of the system via

$$\nu = -\frac{d\epsilon_{xx}}{dP} \left( \frac{d\epsilon_{zz}}{dP} \right)^{-1}$$  \hspace{1cm} (6.3)

which yields 0.224 and 0.228 for the QD and the wire itself respectively. The uniaxial Poisson ratio $\nu^{WZ}$ for WZ materials was previously given in Sec. 2.3.2 by

$$\nu^{WZ} = \frac{C_{13}}{C_{11} + C_{12}},$$  \hspace{1cm} (6.4)
which using the elastic constants from Table. 6.1 results in Poisson ratios of 0.227 and 0.228 for the QD and the wire respectively, in good agreement with what follows from the strain calculations. This proves that the strain distribution for any configuration can be obtained from the built-in strain by simply adding a homogeneous strain to the entire structure defined by the Poisson ratio.

### 6.4 Strain-dependence of the band edges

Using the calculated strain profiles and Eq. 2.32 the position of the band edges can be determined in the NWQD as well as the surrounding barrier. For the conduction band this is shown on a surface in the \( xy \)-plane through the center of the dot in Fig. 6.5a. The conduction band edge appears to be rather homogeneous across the entire QD. Even though the strain distribution spikes near the corners of the hexagon, the conduction band is surprisingly flat, as is emphasized in Fig. 6.5b where the conduction band edge, as well as the valence band edges, are plotted along lines in the \( x \) - and \( y \) -directions through the center of the QD. The flatness of the conduction band edge is attributed to the fact that the spikes in the strain parallel to the \( c \)-axis cancel out the spikes in the strain perpendicular to the \( c \)-axis. This is also true, but to lesser extent, for the three valence bands. It is therefore appropriate to simply use the average strain across the entire dot to describe the band edges in the QD. The band edges along the \( x \)- and \( y \)-directions are identical apart from the fact that the QD is larger in the \( x \)-direction than in the \( y \)-direction due to the hexagonal cross-section. Because of the homogeneity of the band edges across the entire QD and the small difference between the \( x \)- and \( y \)-directions, it is justified to model the QD potential with a cylindrical step function. When inducing a strain along the wire axis of \( \Delta \varepsilon_{zz} \) by stretching or compressing the wire
along the growth direction the total strain $\epsilon_{zz,xx}^{\text{tot}}$ becomes

$$
\begin{align*}
\epsilon_{zz}^{\text{tot}} &= \epsilon_{zz}^{0} + \Delta \epsilon_{zz}, \\
\epsilon_{xx}^{\text{tot}} &= \epsilon_{xx}^{0} - \nu \Delta \epsilon_{zz},
\end{align*}
$$

(6.5)

where $\epsilon_{zz}^{0} = -0.01 \%$ and $\epsilon_{xx}^{0} = -0.60 \%$ are the strain averages across the dot in absence of external force and $\nu$ is the Poisson ratio. Outside the dot $\epsilon_{zz}^{0} = \epsilon_{xx}^{0} = 0 \%$. Using Eq. 2.32 the band edges can now be calculated as a function of the strain induced along the $z$-direction inside and outside the dot (see Fig. 6.6b).

Under the influence of tensile uniaxial strain the top valence band, the HH band, shifts up while the conduction band shifts down, decreasing the band gap by 7 meV at $\Delta \epsilon_{zz} = 0.1\%$. In this case the band gap of WZ is more sensitive to tensile uniaxial strain than the band gap of ZB, which shifts only by 5 meV using ZB parameters and analytically known relations for the ZB band edges [62]. This is mainly due to the lower Poisson ratio of WZ compared to ZB, as the in-plane strains induced by the Poisson effect counteract the energy shift caused by the uniaxial strain. The LH band shifts up as well, while the CH band shifts down, if only slightly. For both the LH and CH bands the separation with the HH band grows with increasing $\Delta \epsilon_{zz}$. Due to the similarity of the deformation potentials of InAs and InP, the shifts of the band edges in the dot barely differ from those in the host.

To calculate the quantization energies, it is relevant to know the barrier height,
Figure 6.6: a) Band diagram for Wurtzite at the $\Gamma$-point b) Shift of the band edges as a function of tensile strain induced in the NWQD for both the InAsP QD (solid lines) and the InP host (dashed lines). c) Change in the barrier height as a function of strain for the CB, HH, LH and CH bands (compared to the unstressed barrier height).

$\Delta V_{\text{barrier}}$, which is obtained from the difference between the band edges inside and outside the QD. For the four bands the barrier heights are $V_{\text{CB, barrier}} = 152$ meV, $V_{\text{HH, barrier}} = 100$ meV, $V_{\text{LH, barrier}} = 79$ meV and $V_{\text{CH, barrier}} = 22$ meV. Their change at $\Delta \epsilon_{zz}$, which is shown in Fig. 6.6c is relatively small, on the order of 0.1 meV.

### 6.5 Quantization energy

A common approach to estimate the electron g-factor in nanostructures, such as a nanowire quantum dot, is to use an adapted Roth formula, where the quantization energy of the electron is added to the energy differences in the denominator [25, 34, 105] to create effective band gaps. In order to calculate the quantization energy a simple numerical model is employed. The QD potential is assumed to be a step function where the barrier height was calculated in Sec. 6.4. This assumption was previously justified in Sec. 6.4, where it was shown that the band edges are homogeneous across the entire dot. Furthermore, the in-plane anisotropy of the QD is disregarded, since the difference between the dot size in the $x$- and $y$-directions is relatively small and the cylindrical symmetry vastly simplifies the calculations.

The model is based on the work of Melnik et al. [130], who established a procedure to calculate the quantization energy in a cylindrically symmetric system with discontinuous mass. Here the procedure is slightly adapted to account for the anisotropic effective mass in WZ structures. The effective mass tensor $m$ is
given by

\[
\mathbf{m} = \begin{bmatrix}
m^\perp & 0 & 0 \\
0 & m^\perp & 0 \\
0 & 0 & m^\parallel 
\end{bmatrix}.
\] (6.6)

In the effective mass approximation, the one-band Schrödinger equation is then given by [131]

\[
-\frac{\hbar^2}{2} \sum_{i,k} \left( \frac{\partial}{\partial x_i} \mathbf{m}_{i,k}(x) \frac{\partial}{\partial x_k} \right) \psi(x) + V(x) \psi(x) = E \psi(x),
\] (6.7)

where \( x \) is the position vector \((x, y, z)\), \( \psi(x) \) and \( E \) are the electron wavefunction and corresponding energy and \( \mathbf{m}(x) \) and \( V(x) \) are the position dependent effective mass tensor and band edge potential energy respectively. Transforming from a cartesian to a cylindrical coordinate system \((x = (\rho, \phi, z))\), the \( \phi \)-coordinate can be separated from \( \psi \) via

\[
\psi(x) = \chi(\rho, z) \Phi(\phi)
\] (6.8)

since the system is assumed to have cylindrical symmetry. It is important to note that since in a WZ system the effective mass is isotropic in-plane, the effective mass tensor remains unchanged when transforming it to a cylindrical coordinate system. Equation 6.7 then becomes

\[
-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \left( \frac{1}{m^\parallel(\rho, z)} \frac{\partial \chi}{\partial z} \right) \Phi(\phi) - \frac{\hbar^2}{2} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \frac{\rho}{m^\perp(\rho, z)} \frac{\partial \chi}{\partial \rho} \right) \Phi(\phi)
\]

\[
- \frac{\hbar^2}{2m^\perp(\rho, z)} \frac{\chi(\rho, z)}{\rho^2} \frac{\partial^2 \Phi}{\partial \phi^2} + V(\rho, z) \chi(\rho, z) \Phi(\phi)
\] (6.9)

\[
= E \chi(\rho, z) \Phi(\phi).
\]

Dividing by \( \chi(\rho, z) \Phi(\phi) \), multiplying with \( m^\perp(\rho, z) \rho^2 \) yields

\[
\frac{m^\perp(\rho, z) \rho^2}{\chi(\rho, z)} \left( -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \left( \frac{1}{m^\parallel(\rho, z)} \frac{\partial \chi}{\partial z} \right) - \frac{\hbar^2}{2} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \frac{\rho}{m^\perp(\rho, z)} \frac{\partial \chi}{\partial \rho} \right) \right)
\]

\[
+ m^\perp(\rho, z) \rho^2 (V(\rho, z) - E) = \frac{\hbar^2}{2} \frac{\partial^2 \Phi}{\partial \phi^2} \frac{1}{\Phi(\phi)} \equiv -\frac{\hbar^2}{2} n^2.
\] (6.10)

The equation for \( \Phi(\phi) \) has obvious solutions of the form

\[
\Phi(\phi) = e^{in\phi}
\] (6.11)

where \( n \) is an integer in order to have \( \Phi(0) = \Phi(2\pi) \). The rest of the equation can be rewritten as

\[
-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \left( \frac{1}{m^\parallel(\rho, z)} \frac{\partial \chi}{\partial z} \right) - \frac{\hbar^2}{2} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \frac{\rho}{m^\perp(\rho, z)} \frac{\partial \chi}{\partial \rho} \right)
\]

\[
+ \frac{\hbar^2}{2} \frac{n^2}{m^\perp(\rho, z) \rho^2} \chi(\rho, z) + V(\rho, z) \chi(\rho, z) = E \chi(\rho, z).
\] (6.12)
This is a partial differential equation (PDE) which can be solved using a finite element method in Comsol. Using the naming conventions of Comsol, the PDE can be written in coefficient form as

\[
\nabla \cdot (-c \cdot \nabla \chi) + a \chi + \beta \cdot \nabla \chi = \delta \alpha \lambda \chi
\]

where the coefficients are given by

\[
c = \frac{\hbar^2}{2} \begin{bmatrix}
\frac{1}{m^\perp} & 0 \\
0 & \frac{1}{m^\parallel}
\end{bmatrix}, \quad a = \frac{\hbar^2 n^2}{2 \rho^2 m^\perp} + V, \quad \beta = -\frac{\hbar^2}{2 \rho} \begin{bmatrix}
\frac{1}{m^\parallel} & 0 \\
0 & 0
\end{bmatrix}
\]

and \( \delta \alpha = 1 \). \( \lambda \) is the eigenvalue of the system which in this case is equal to the quantization energy \( E \). Note that the term \( \beta \) arises from the peculiar convention in Comsol that the divergence operator in cylindrical coordinates is defined as \( \frac{\partial \chi}{\partial \rho} + \frac{1}{\rho} \frac{\partial \chi}{\partial z} \) rather than the conventional \( \frac{1}{\rho} \frac{\partial (\rho \chi)}{\partial \rho} + \frac{\partial \chi}{\partial z} \).

The coefficients of Eq. 6.14 are incorporated in a 2D axisymmetric model. The QD is defined as a rectangle with height \( h = 5 \) nm and width \( r = 10 \) nm. The potential \( V \) is set to zero inside the QD, and to the previously calculated \( V \) barrier outside the QD. Effective masses of InAs\(_{0.3}\)P\(_{0.7}\) and InP as given in Table 6.1 are assigned to the QD and the host respectively. Boundary conditions are enforced on the border of the QD to enforce the continuity of \( \chi(\rho, z) \), \( \frac{1}{m^\parallel(\rho, z)} \frac{\partial \chi}{\partial \rho} \) and \( \frac{1}{m^\perp(\rho, z)} \frac{\partial \chi}{\partial z} \). Using the effective masses and barrier height for the respective band, the quantization energy in each of the bands is calculated separately.

The quantization energies in the conduction band and the three valence bands are 73 meV, 19 meV, 32 meV and 19 meV respectively. The change of the quantization energies at \( \Delta \epsilon_{zz} = 0.1\% \) is on the order of 10 \( \mu \)eV and can be disregarded. The quantization energy will be assumed constant. By adding the quantization energies of the conduction band and the top valence band to the band gap energy the emission energy is calculated to be 1.330 eV. This decreases to 1.323 eV at \( \Delta \epsilon_{zz} = 0.1\% \).

### 6.6 Electron g-factor in WZ materials

The Roth formalism follows from second-order \( k \cdot p \)-perturbation theory [9] and was developed to describe the electron g-factor in ZB bulk materials. When applied to the ZB basis functions given in Table 2.3 the Roth formalism results in a compact equation given by

\[
g_{\text{Roth}} = 2 - \frac{2E_P \Delta}{3E_g(E_g + \Delta)},
\]

which depends only on the band gap \( E_g \), spin-orbit coupling \( \Delta \) and the Kane energy \( E_P \) which is related to the momentum matrix element involving s- and
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

$p$-like Bloch functions. The Roth formula in Eq. 6.15 is able to accurately predict the electron g-factor in bulk III-V semiconductors. Analogous to the derivation of the Roth formula for ZB, the out-of-plane electron g-factor $g_{e,z}$ for WZ materials can be calculated using

$$g_{e,z} = g_0 \left(1 - \frac{i}{m_0} \sum_{\delta} \frac{\langle \gamma | p_x | \delta \rangle \langle \delta | p_y | \gamma \rangle - \langle \gamma | p_y | \delta \rangle \langle \delta | p_x | \gamma \rangle}{E_\gamma - E_\delta} \right),$$

(6.16)

where $g_0$ is the free electron g-factor with a value of 2, $\gamma$ is the band for which the g-factor is to be calculated and $\delta$ sums over all other bands. It is sufficient to only consider the bottom conduction band and the top three valence bands. Using $\gamma = iS \uparrow$ and the basis functions for WZ given in Table 2.3 one finds different contributions from the different valence bands and $g_{e,z}$ can be written as

$$g_{e,z} = 2 + g_{HH} + g_{LH} + g_{CH},$$

(6.17)

where

$$g_{HH} = -\frac{1}{E_A} E_{P2}, \quad g_{LH} = \frac{a^2}{E_B} E_{P2} \quad \text{and} \quad g_{CH} = \frac{b^2}{E_C} E_{P2}$$

(6.18)

are the contributions from the three different valence bands to $g_{e,z}$. In Eq. 6.18 $E_{P2} = 2 \langle iS | p_x | X \rangle^2 / m_0$ is the Kane energy relating $\langle S \rangle$ and $\langle X \rangle$, $E_A$, $E_B$ and $E_C$ are the energy separations between the conduction band and the heavy hole band, light hole band and crystal field split hole band respectively, and $a$ and $b$ are normalization constants which mix the LH and CH bands defined in Eq. 2.34. The out-of-plane electron g-factor $g_{e,z}$ arises from an interplay between all three valence bands, where the HH band has a negative contribution and the LH and CH bands have counteracting positive contributions. Due to the energy difference in the denominator and the fact that $a^2 + b^2 = 1$, the contribution of the HH band is always larger than the contribution of the other two valence bands combined, which leads to a net negative contribution and $g_z < 2$.

Contrary to ZB materials, where in bulk the g-factor is isotropic and anisotropy in the g-tensor is only obtained when considering confinement in nanostructures, the g-tensor for WZ materials is already anisotropic due to the anisotropic crystal structure. One can adjust Eq. 6.16 to account for a magnetic field applied perpendicular to the $c$-axis of the WZ material according to [102]

$$g_{e,x} = g_0 \left(1 - \frac{i}{m_0} \sum_{\delta} \frac{\langle \gamma | p_y | \delta \rangle \langle \delta | p_z | \gamma' \rangle - \langle \gamma | p_z | \delta \rangle \langle \delta | p_y | \gamma' \rangle}{E_\gamma - E_\delta} \right),$$

(6.19)

where $\gamma'$ denotes band $\gamma$ with opposite spin. Due to the absence of $\langle Z \rangle$ in the basis functions for the heavy hole band, the contribution of the HH band is zero.
and only contributions from the LH and CH bands remain, such that

\[ g_{e,x} = 2 + g_{LH} + g_{CH}, \]  

(6.20)

where

\[ g_{LH} = -\sqrt{2} \frac{ab}{E_B} \]  

and

\[ g_{CH} = \sqrt{2} \frac{ab}{E_C}. \]  

(6.21)

In Eq. 6.21 \( E_P^1 = \frac{2 \langle iS | p_z | Z \rangle^2}{m_0} \) is the Kane energy relating \( \langle S \rangle \) and \( \langle Z \rangle \). The negative contribution of the LH band to \( g_{e,x} \) outweighs the positive contribution of the CH bands and \( g_{e,x} < 2 \). The in-plane electron g-factor \( g_{e,x} \) in WZ is fundamentally different from the out-of-plane electron g-factor \( g_{e,z} \) as it arises from the interplay between only the LH and CH bands, rather than from all three valence bands. The Kane energies \( E_P^1 \) and \( E_P^2 \) are in general not equal to each other. Even though they are not experimentally known for WZ III-V’s, they can be calculated using [132]

\[ E_P^1 = \left( \frac{m_0}{m_e^\parallel} - 1 \right) \frac{(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2}{E_g + 2\Delta_2}, \]  

(6.22)

\[ E_P^2 = \left( \frac{m_0}{m_e^\perp} - 1 \right) \frac{E_g((E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2)}{(E_g + \Delta_1 + \Delta_2)(E_g + \Delta_2) - \Delta_3^2}, \]  

(6.23)

where \( \Delta_1 = \Delta_{cf} \) and \( \Delta_2 = \Delta_3 = \Delta_{so}/3 \). Using the parameters given in Table 6.1, this yields \( E_P^1 = 15.4 \) eV and \( E_P^2 = 11.4 \) eV for InP and \( E_P^1 = 17.1 \) eV and \( E_P^2 = 12.9 \) eV for InAs. These results are comparable to those in Ref. [107], where the Kane energies were determined by fitting an eight-band \( k \cdot p \)-model to an ab initio band structure. For both materials it is found that \( E_P^1 > E_P^2 \). The same anisotropy has also been predicted for GaN and InN [133]. The values for the Kane Energies in WZ are significantly lower compared to their ZB counterparts (InP: \( E_P = 20.7 \) eV, InAs: \( E_P = 21.5 \) eV) which supports the previous notion that in general the electron g-factors for WZ are higher than those of ZB. The electron g-factors can be calculated using

\[ g_{e,z} = 2 - \left( \frac{1}{E_A} - \frac{a^2}{E_B} - \frac{b^2}{E_C} \right) E_P^2, \]  

(6.24)

\[ g_{e,x} = 2 - \left( \frac{\sqrt{2}ab}{E_B} - \frac{\sqrt{2}ab}{E_C} \right) \sqrt{E_P^1 E_P^2}. \]  

(6.25)

When the bracketed terms in \( g_{e,z} \) and \( g_{e,x} \) become comparable in magnitude, which is the case for InP, the anisotropy of the electron g-tensor is determined by the anisotropy of the Kane energies. One finds \( g_{e,z} = 1.58 \) and \( g_{e,x} = 1.53 \) for InP and \( g_{e,z} > g_{e,x} \) because \( E_P^1 > E_P^2 \). For InAs the bracketed terms in \( g_z \) and \( g_x \) differ
substantially and the opposite anisotropy is found: \( g_{e,z} = -5.27 < g_{e,x} = -4.92 \). This leads to the question what will happen for the InAs\(_{0.3}\)P\(_{0.7}\) alloy which the QD is composed of. The electron g-factors for different InAsP alloys are shown in Fig. 6.7. The electron g-factor anisotropy switches at high As-concentrations. At an As-concentration of 30 \%, \( g_{e,z} = 1.08 > g_{e,x} = 1.01 \).

Experimental values for the in-plane electron g-factor for InP are reported as \( g_{e,x} = 1.4 \) [98] and \( g_{e,x} = 1.3 \) [99], agreeing well with the value obtained here. The g-factors for WZ InAs are not readily available, however one experiment performed on InAs nanowire quantum dots suggests that the g-factor for WZ InAs approaches that of ZB InAs (-14.7 [14]) in the bulk limit [105]. This contradicts the calculations presented here, as a much smaller deviation from the free electron g-factor is found. Unrealistically large Kane energies would be required to bring the WZ InAs g-factors towards the ZB values. It should be stressed that the Kane energies merely renormalize the g-factors and their strain-dependencies. The trends observed later in this chapter will therefore be independent of the choice of Kane energies.

### 6.7 Strain-dependence of the electron g-factor

Using Eqs. 6.18 and 6.21 and replacing the energy differences with the quantization energies calculated in Sec. 6.5 added to the strain-dependent energy differences calculated in Sec. 6.4, the in-plane and out-of-plane electron g-factors of the InAsP QD can be calculated. This results in \( g_{e,z} = 1.21 \) and \( g_{e,x} = 1.27 \) when only the built-in strain due to lattice mismatch is present. Size quantization affects \( g_{e,x} \) more than \( g_{e,z} \) and the anisotropy is reversed compared to bulk InAsP. This reversal of anisotropy has been observed in crystal phase InP QDs [134]. It should be stressed that even though the model presented here takes into account quantiza-
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

Figure 6.8: a) Contributions of the three valence bands to $g_{e,z}$ as a function of tensile strain. b) Contributions of the second and third valence bands to $g_{e,x}$ as a function of tensile strain. c) $g_{e,z}$ (in black) and $g_{e,x}$ (in red) as a function of tensile strain. They are obtained by adding the contributions shown in a) and b) to the free electron g-factor which has a value of 2.

With increasing strain the band edges shift and the contribution of each of the valence bands to the electron g-factors changes. The contribution from the LH band to $g_{e,z}$ increases, while the contributions from the HH and CH bands decrease as is illustrated in Fig. 6.8a. The result is a small decrease in $g_{e,z}$ with increasing strain $\Delta \epsilon_{zz}$. For $g_{e,x}$ the responses to strain of the two valence bands counteract one another and result in a small decrease of $g_{e,x}$. The strain-sensitivities of $g_{e,z}$ and $g_{e,x}$ are given in Table 6.3 and are normalized to the sensitivity of the emission energy to later compare the results obtained here with the experiment presented in Ch. 7.

6.8 Valence band g-factors

While remote bands can safely be neglected for the electron g-factor, the same assumption does not hold for the valence band. The complex nature of the valence band makes it more challenging to form an intuitive picture. The valence band
in an external magnetic field was first treated by Luttinger [69] and led to the introduction of two phenomenological parameters $\kappa$ and $q$, where $\kappa$ determines the Zeeman splitting linear in $J$, while $q$ determines the Zeeman splitting cubic in $J$. The in-plane and out-of-plane hole g-factors are [67]

$$g_{h,x} = 3q, \quad g_{h,z} = 6\kappa + \frac{27}{2}q. \tag{6.26}$$

The term cubic in $J$, $q$, is often omitted as its contribution is negligible compared to $\kappa$. Known values for the magnetic Luttinger parameters for ZB are $\kappa = 7.68$, $q = 0.04$ for InAs and $\kappa = 0.97$, $q = 0.02$ for InP [63]. In the approximation of $q = 0$, $g_{h,x}$ for a heavy hole (and its sensitivity to strain) becomes zero, while $g_{h,z}$ for a heavy hole is equal to $g_{h,z} = 6\kappa$ [135]. It can be shown that in the quasi-cubic approximation these relations are also valid for WZ [104]. For the cubic ZB crystal the $z$-axis is only defined in the presence of a magnetic field and one always probes $g_{h,z}$ independent of which principal axis the magnetic field is applied along. For the hexagonal WZ crystal this is fundamentally different, as in bulk the $z$-axis is intrinsically defined by the anisotropy of the crystal structure. The sign of the hole g-factor is defined in the same way as in Chs. 4 and 5. It should be noted that in literature the opposite definition is also sometimes encountered.

In a bulk WZ semiconductor the top-most valence band is the heavy hole band, which mixes with the other valence bands. To calculate the g-factor of the hole ground state, the coupling with other bands has to be carefully considered. An approach to accomplish this was formulated for WZ GaN by Rodina et al. [104]. In bulk, $g_{h,z}$ deviates from $6\kappa$ due to a magnetic field induced coupling between the HH band and the LH and CH bands. Taking this coupling into account results in [104]

$$g_{h,z} = 6\kappa - \frac{96}{5} \frac{\mu_0}{m_0} \gamma^2 \left( (4a^2 + \eta b^2) M \left( \frac{E_{AB}}{R_0} \right) + (4b^2 + \eta a^2) M \left( \frac{E_{AC}}{R_0} \right) \right), \tag{6.27}$$
Chapter 6. Strain and g-tensors in an InAsP nanowire quantum dot

Figure 6.9: a) Valence band splittings $E_{AB}$ and $E_{AC}$ as a function of induced strain $\Delta \epsilon_{zz}$. The separation of the HH band with both the LH and CH bands increases with strain. b) Out-of-plane hole g-factor as a function of strain.

where $M(x)$ is a universal function defined in the Appendix of Ref. [104], $m_0$ is the rest mass of the electron, $\mu_0$ is the average exciton reduced mass, $\eta = \epsilon_0^\perp/\epsilon_0^\parallel$ is the ratio between the in-plane and out-of-plane dielectric constants, $a$ and $b$ are the normalization constants responsible for the mixing between the LH and CH subbands previously defined in Eq. 2.34 and $\gamma = \gamma_2 = \gamma_3$ is the Luttinger parameter in the spherical approximation. For WZ InP and InAs the dielectric constants are not known and are assumed to be equal to the values for ZB, $\epsilon_0 = \epsilon_0^\perp = \epsilon_0^\parallel = \epsilon_{0ZB}$, which are $\epsilon_0 = 15.5$ and $\epsilon_0 = 12.5$ for InAs and InP respectively. This simplification holds well for GaN and as a consequence $\eta = 1$. Finally the arguments of $M(x)$ are the energy separations between the HH band and the LH ($E_{AB}$) and CH ($E_{AC}$) bands divided by the effective Rydberg energy $R_0 = \mu_0 e^4/2\hbar^2\epsilon_0^2$. For InP this leads to $g_{h,z} = 4.2$. Combined with the calculated value for the out-of-plane electron g-factor, $g_{e,z} = 1.21$, this is in good correspondence with $|g_{e,z} - g_{h,z}| = 3.5$ and $|g_{e,z} - g_{h,z}| = 4.66$ reported in literature [98, 99].

In a nanostructure the contribution determined by $\kappa$ is expected to quench [25] and size quantization heavily affects the degree of mixing between the light and heavy holes [86]. Applying Eq. 6.27 to the InAsP QD directly, with the use of previously calculated strain and quantization energies, leads to a hole g-factor of $g_{h,z} = 11.8$. Hole g-factors of this magnitude are realistically not observed in QDs. The quenching caused by the confining potential of the nanostructure renormalizes the contribution from the remote bands, which has to be taken into account to accurately determine the hole g-factor in a nanostructure. A method to implement this was recently presented by Semina and Suris [86].

However, the strain-dependence of the hole g-factor can still be estimated by taking the remote band contribution to be independent of strain, which is a fair assumption since strain does not affect the confining potential of the investigated WZ InAsP QD. The strain-dependence is then determined by the mixing of the light hole and crystal field split hole into the valence band ground state and can
be calculated with the second term in Eq. 6.27. The result is plotted in Fig. 6.9b. Because the separation of the HH band with both the LH and CH bands increases, as shown in Fig. 6.9a, \( g_{h,z} \) also increases. The same behaviour was found for the self-assembled QDs in Chs. 4 and 5, where an increase of \( g_{h,z} \) was found with increasing HH-LH splitting. Analogous to the self-assembled dots, the sensitivity of \( g_{h,z} \) (see Table 6.3) is much larger than the sensitivity of the electron g-factors.

6.9 Conclusions

This chapter has introduced a model to calculate the (strain-dependence of the) electron and hole g-factors in WZ nanostructures. An extensive discussion of relevant parameters for WZ InAs and InP was given. The strain distribution in the NWQD was calculated using a finite element method in Comsol Multiphysics. Using the calculated strain distribution the position of the band edges of the conduction band and the three valence bands in the entire structure was calculated. Even though the strain distribution itself is inhomogeneous near the corners of the hexagonal cross-section of the QD, the in-plane and out-of-plane components of the strain cancel each other out and the band edges were found to be constant across the entire QD. This observation validated the use of a step function to model the QD potential to calculate quantization energies in the different bands. Quantization energies were calculated assuming cylindrical symmetry in a one-band effective mass approximation with discontinuous mass solved using a finite element method in Comsol Multiphysics.

Using the relations for the electron g-factors in bulk WZ materials, the g-factors for InAsP were calculated. For pure InP the calculated values of \( g_{e,z} = 1.58 \) and \( g_{e,x} = 1.53 \) were obtained. The value of \( g_{e,x} \) is in good agreement with available experimental data. At high As-concentration the anisotropy of the electron g-factor reverses and for pure InAs \( g_{e,z} = -5.27 \) and \( g_{e,x} = -4.92 \). Because the electron g-tensors for WZ InAs and InP have, as of yet, not been disentangled, the results presented here cannot be fully compared with experimental data. Determining the complete electron g-tensor by performing g-factor measurements in different orientations of the magnetic field would be a worthwhile test and can help to establish more reliable parameters for the momentum matrix elements.

The calculated quantization energies on top of the strain-dependence of the band edges were used to calculate the in-plane and out-of-plane electron g-factors for an InAsP NWQD via the adapted WZ Roth formula, resulting in \( g_{e,z} = 1.21 \) and \( g_{e,x} = 1.27 \). Both components experience a small decrease when the NWQD is exposed to tensile strain. For the self-assembled QDs in Chs. 4 and 5 it was found
that the sensitivity of the electron g-factors was dominated by the confinement energy which affected the quenching of the orbital momentum. For the WZ NWQDs this mechanism can be ruled out since the barrier height, and consequently the confinement energy, is barely affected by tensile strain. Instead the sensitivity of the electron g-factors arises solely from a shift of the band edges which affects the contributions of the different bands to $g_{e,z}$ and $g_{e,x}$, resulting in a net decrease of both components.

The strain-dependence of the hole g-factors was estimated based on the work of Rodina et al. [104]. Disregarding terms cubic in $J$, the in-plane hole g-factor $g_{h,x} = 0$ and insensitive to strain. The out-of-plane hole g-factor was calculated to be $g_{h,z} = 4.2$ for InP, in good agreement with experimental observations. By disregarding the quenching of the remote band contributions, which can be assumed to be constant as strain does not affect the confining potential, the strain-dependence of $g_{h,z}$ was calculated. An increase of $g_{h,z}$ with increasing strain was found, caused by the increased splitting between the HH band and the LH and CH bands. The same dependence was found for the self-assembled dots in Chs. 4 and 5. In the next experiments on InAsP NWQDs are described, of which the results can be used to test the calculations presented in this chapter.
Chapter 7

Magneto-optical characterization of a strained nanowire quantum dot

To be published.
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

7.1 Introduction

In this chapter a new method will be developed to apply uniaxial stress to nanowire quantum dots (NWQDs) which is then used to investigate the strain-dependence of the electron and hole g-tensors in these NWQDs. Sophisticated microelectromechanical systems (MEMS) exist which can successfully be employed to generate large strains of 1% and higher in nanowires, even up to the breaking point of the wire. These MEMS are for example based on electrostatically driven comb-drive actuators [136] or strain-amplifying piezoelectric actuators [96] and often rely on geometrically large structures in order to strain a single nanowire.

A more simple and straightforward approach is to place a nanowire directly on the surface of a piezoelectric actuator, which is the method used for the work presented in this chapter. A major advantage of this approach is that it takes place on a much smaller scale than the aforementioned MEMS. Micromachining makes it possible to define piezoelectric structures on a micrometer scale [137]. A disadvantage is the lower amount of strain that can be induced, since it is limited by the piezoelectric material.

Fabrication of the device will be described in Sec. 7.2 followed by the characterization of the device in 7.3. The characterization will focus on the dependence of the photoluminescence on externally induced strain and identification of the different peaks that are observed in the PL spectra.

Results from the magneto-optical measurements, which are performed in three different geometries to extract the electron and hole g-tensors, are presented in Sec. 7.4. Finally, Sec. 7.5 discusses how to resolve the full g-tensor and elaborates on its strain-dependence.

7.2 Sample fabrication

The device employed for the experiments presented throughout this chapter consists out of CBE-grown InAsP/InP nanowire quantum dots, mounted across a gap etched in a PMN-PT piezoelectric substrate. The fabrication process will be addressed step by step.

7.2.1 Nanowire growth

The nanowires were grown by D. Dalacu at the University of Ottawa, Canada. The growth process will be briefly summarized here; full details can be found in Ref. [138].

Using an electron beam and subsequent wet etching with buffered HF, an array
of holes is defined in a 20 nm SiO$_2$ mask on top of a (111)B S-doped InP substrate. The size of these patterned holes defines the diameter of the gold catalyst, which serves as a good estimate of the quantum dot diameter.

The gold catalyst is deposited everywhere and then left behind in the center of the hole in a metal lift-off process. Using chemical beam epitaxy (CBE), with trimethylindium (TMI) and PH$_3$ as precursor, the InP core is first grown. At the desired height, PH$_3$ is briefly exchanged for AsH$_3$, embedding a QD in the nanowire core with a height depending on the time of exposure to AsH$_3$. Finally, by raising the growth temperature, an InP shell is grown around the core.

The growth procedure used for the wires discussed in this chapter differs from the one presented in Ref. [138] in several ways. The introduction of AsH$_3$ was delayed to grow the dot roughly halfway in the wire, rather than in the bottom. This is necessary to ensure the quantum dot is located above the gap etched in the piezo. This procedure was found to introduce many stacking faults in and near the QD, deteriorating the quality of the emission. This was overcome by greatly reducing the growth rate at the height of the QD.

The wires were originally designed to have high emission in the growth direction of the nanowire. Due to the geometry of the experiment presented in this chapter, where the wires are always excited and collected from perpendicular to the nanowire growth direction, high radial emission is more desirable. To achieve this, the amount of tapering at the end of the wire was reduced.

The quantum dots are estimated to have a diameter of 20 nm, a height of 3-5 nm and an As concentration of 30%. The thickness of the InP shell is ±100 nm. These parameters were also used for the calculations presented in Ch. 6. Figure 7.1 shows a Scanning Electron Microscopy (SEM) image of the grown nanowire array.
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

PMN-PT, Au SiN InP Pt
Top view
Side view

Figure 7.2: a) and b) Schematic representations of the top and side views of the finalized device. c) and d) Scanning electron microscopy images of the device before and after deposition of the Pt contacts.

7.2.2 Nanowire transfer

In order to apply stress to a nanowire using a piezoelectric actuator, the simplest approach would be to directly place it on top of the piezoelectric actuator. Applying a voltage to the piezoelectric substrate then results in additional strain in the nanowire due to the Van der Waals force fixing the wire to the surface. This approach was applied by Chen et al. [139] and resulted in a blue-shift of the QD emission of roughly 3 meV. However, using this approach the generated strain field becomes unpredictable as the entire wire is in contact with the piezoelectric surface. Furthermore, full transfer of the strain from the piezoelectric actuator to the wire is not guaranteed. This was recently demonstrated by Elshaari et al. [140], who showed a fourfold increase in the tunability of the emission energy when comparing a device with and without the wire directly fixed to the surface. However, in this work the maximum tunability was still limited to less than 3 meV. In an attempt to improve on this, in the current work the wires are placed and fixed across holes in the piezo-electric actuator.

PMN-PT, which was already introduced in Ch. 5, is the used piezoelectric material. The top of the actuator is coated with a 200 nm thick gold layer. Using Inductively Coupled Plasma Chemical Vapour Deposition (ICPCVD) a 100 nm thick SiN layer is deposited on top of the gold to act as an insulating layer. Next,
four 5×5 µm, 200 nm deep holes are etched away using a Focused Ion Beam (FIB). Using a nanomanipulator in a SEM, one by one a wire is picked up from the nanowire sample and placed across one of the gaps. Finally, using the FIB, each wire is fixed to the SiN surface by depositing Platinum at both ends. A schematic representation and image of the final structure is found in Fig. 7.2. The presence of the hole ensures a purely uniaxial strain along the growth direction of the QD. Any strain in the perpendicular direction is localized close to the clamping points due to the high aspect ratio of the wire and not present in the NWQD. The Pt-contacts ensure a full strain transfer from the piezoelectric actuator to the nanowire. This should increase the maximum amount of strain that can be generated in the wire to the limit of the used piezoelectric actuator, which is around 0.5 %.

Before use the device needs to go through a poling procedure to align the piezoelectric domains, as was previously described in Sec. 5.2.1. In this case the actuator is poled in such a way that application of a positive voltage results in a tensile strain in the nanowire.

### 7.3 Sample characterization

The characterization setup described in Sec 3.2 is used to measure the photoluminescence spectra of several single nanowires, before transfer to the device. This is necessary to select the wires most suitable for the magneto-luminescence experiment in terms of PL intensity and linewidth. The lines need to be narrow enough so they can be resolved when they split up when a magnetic field is applied.

Even though the yield of suitable nanowires is quite high (>50 %), the transfer from the nanowire array to the piezoelectric actuator is not always successful and several wires are lost in the process. Therefore a total of forty single wires were characterized to ensure a sufficient number of wires could be transferred to the device.

PL spectra of the four wires (A, B, C and D) that were in the end transferred to the device are shown in Fig. 7.3, where the fifth spectrum shows an example of a less suitable wire (E). To increase visibility the spectra have been normalized. In Fig. 7.3a, three different regions in the PL spectrum are distinguished. Region I shows a small peak which corresponds to the emission of the WZ InP nanowire. Averaging over all forty nanowires yields a peak position of 1.4940±0.0002 eV, which is in good agreement with the band gap of bulk WZ InP found in literature [115]. Region II consists of a broad emission with some sharp features ranging from 1.35 eV all the way up to 1.48 eV. These features are related to crystal defects in the nanowire, such as stacking faults [109, 141].
Figure 7.3: a) Normalized photoluminescence spectra of the four nanowires of the final experiment, plus a fifth wire showing less suitable emission. Three different areas corresponding to the PL from the WZ InP wire (I), the defects in the wire (II) and the QDs themselves (III) are indicated. b) Enlarged view of the QD emission of the same wires as shown in a), recorded with a higher resolution grating.

Region III shows the QD emission, between 1.27 eV and 1.31 eV. In Ch. 6 the emission energy of a typical InAsP QD was calculated to be 1.33 eV, close to the QD emission observed here. The small discrepancy can easily be accounted for by a variation of dot parameters. The intensity of the QD emission ranges from 500 to 1000 counts per second, although it should be noted that due to the large number of wires to be characterized the PL emission was not optimized for each wire and the maximum intensity is likely to be higher. Each dot has several spectral lines, corresponding to different excitonic complexes. Figure 7.3b shows the QD emission of the same wires recorded with a higher resolution grating. For the four transferred wires the QD linewidth is $<100 \mu$eV, corresponding to the resolution of the spectrometer. The fifth wire shows a much larger linewidth, making it unsuitable for the magneto-luminescence experiment.

Exposure of nanowires to an electron beam is known to significantly affect the photoluminescence of nanowires in a negative manner [142]. The mechanism behind this is not precisely known but is usually ascribed to incorporation of carbon in or on the surface of the nanowire [143]. In the present experiment exposure of the wires to an electron beam is inevitable and occurs during several steps in the device fabrication. However, the PL spectra in Fig. 7.3 were recorded after exposure of the wire to the SEM. Comparison of the spectra with wires that
were not exposed to the SEM reveals that the emission of the QDs is unaffected by the SEM, both in terms of linewidth and intensity. The WZ InP peak, which remains at 1.494 eV, reduces in intensity by at least one order of magnitude. This indicates that the WZ InP shell is heavily affected by exposure to the electron beam, while it serves as a protective layer around the QD.

### 7.3.1 Peak-identification

For the remainder of this chapter, analysis will focus on wire A and is then extended to the other wires. As mentioned before, each spectrum usually contains multiple lines originating from different excitonic complexes. In order to fully describe the behaviour of each of these spectral lines when exposed to an external magnetic field or strain, identification of each of these lines is crucial.

The exciton and biexciton can be distinguished by investigating the dependence of the line intensity on the excitation density. In the unsaturated regime the exciton should exhibit a linear dependence on the excitation density, while the biexciton should, under ideal circumstances, exhibit a quadratic dependence according to rate equations [144, 145]. In some cases the biexciton fails to meet these ideal circumstances due to a reduced carrier capture rate into the dot at higher occupancies [146], resulting in a less than quadratic (but more than linear) dependence.

To identify the different excitonic complexes, Fig. 7.4a shows the PL spectrum of wire A for different excitation densities. Note that each subsequent spectrum is given a small offset in the $x$-direction to increase the visibility of the figure. In reality the excitation density dependence of the peak position is small, red-shifting the spectrum roughly 40 $\mu$eV from the lowest excitation density shown in Fig. 7.4a to the highest, possibly due to heating effects which have been reported to red-shift the PL of bulk WZ InP [112]. The intensity of the three lines which are already present at relatively low excitation densities - which will also be the lines subject to investigation in the remainder of this chapter - is plotted on a double logarithmic scale as a function of excitation density in Fig. 7.4b. The intensity of each line saturates at higher excitation densities. The data is fitted with an $ax^b$ dependency in the unsaturated regimes. For the highest energy peak this yields a slope of 1.01, identifying it as the neutral exciton $X^0$, while the middle energy peak shows a slope of 1.98, which is the ideal value for the biexciton $XX$. The third peak, at the lowest energy, shows a slope of 1.21 and is therefore most likely related to a charged exciton. The exciton can be either positively or negatively charged. In work on similar InAsP QDs the peak was identified to be negatively charged [147] and it seems likely that this identification is also valid here. Since it
Figure 7.4: a) Photoluminescence spectrum of wire A for various excitation densities. b) double logarithmic plot of the PL intensity of the three principal lines as a function of the excitation density. The numbers give the exponential factor $b$ when the data is fit with $ax^b$ in the unsaturated regime. Combined with the magnetic field dependent measurements presented later in the chapter this leads to the identification of the peaks as indicated in the figure.

is not essential to distinguish between either positively or negatively charged, the charged exciton is denoted by $X^*$. To further distinguish between the neutral exciton $X^0$ and the charged exciton $X^*$ and confirm their identification, the exchange interaction has to be considered. As argued in Sec. 2.6, the charged exciton does not exhibit any exchange splitting. From the magnetic field dependent measurements presented in Sec. 7.4 it will become clear that the lowest energy peak does not show any exchange splitting, while the other two do, hence verifying the identification as shown in Fig. 7.4.

### 7.3.2 Strain characterization

After transfer and mounting of the wires onto the piezoelectric actuator, the device is poled and subsequently cooled down to liquid helium temperature (4 K). By applying a voltage opposite to the poling direction, a tensile strain is generated in the entire device and transferred to the wire. The choice for tensile strain is made since compressive strain may cause the wires to bend rather than compress, leading to an inhomogeneous and unpredictable strain field. Eventually the wire could even break.

The PL spectrum of wire A as a function of the voltage applied to the piezoelectric actuator is shown in Fig. 7.5. Without biasing the piezoelectric actuator, the PL is compared with the spectrum recorded before transfer of the wire to
the device (in red). A small red-shift of roughly half a meV is observed, which is not unexpected due to a pre-strain caused by mounting and cooling down of the device as PMN-PT and WZ InP are expected to have similar but different thermal expansion coefficients [148, 149]. When applying a tensile stress to the wire a red-shift of the peaks is observed. From the peak positions plotted in the right panel it is clear they do not follow a linear behaviour; instead they can be fit with a quadratic polynomial. This non-linearity was also observed by Chen et al. [139], where it was blamed on the imperfect anchoring of the wire. This is a reasonable explanation, as the only other option, namely that the emission energy depends non-linearly on the induced strain, is not very likely since the amount of strain induced in the QD is still a perturbation compared to the amount of built-in strain already present due to lattice mismatch between the QD and the wire. The suggestion that the non-linearity has a mechanical origin instead and is for example caused by the Pt contacts is confirmed when sweeping the voltage from 200 V back to 0 V, which reveals a small hysteresis.

Comparison of the coefficients, which are equal for the three peaks within their uncertainty (<0.5 %), reveals that the different excitonic complexes do not behave differently when exposed to tensile stress. The QD emission shows a red-shift of 4.6 meV at the maximum applied voltage of 200 V. Wires B, C and D show the

Figure 7.5: a) Photoluminescence spectra of wire A as a function of the voltage applied to the piezo-electric actuator. At 0V the spectrum is compared to the one recorded for the same wire before the transfer, showing a small red-shift (in red). b) Peak positions as a function of the applied voltage, showing non-linear behaviour identical for the three distinguishable peaks.
same non-linear behaviour, with red-shifts of 2.5, 3.8 and 4.7 meV respectively. The unexpectedly large dot-to-dot variations may be ascribed to differences in mounting or the position of the QD with respect to the Pt contact. The applied voltage is in this case limited by the electronics of the used setup rather than the device itself. The observed energy shifts already exceed the ones reported in Refs. [139] and [140] and can increase to 15-20 meV at the maximum operating voltage of the device, provided that the wire doesn’t break. According to the calculations in Ch. 6, a shift of 20 meV corresponds to a strain of roughly $\Delta \epsilon_{zz} = 0.3\%$. Experiments performed using more sophisticated microelectromechanical systems (MEMS) [136] performed on Germanium [150] and Gallium Phosphide [151] nanowires have yielded strain levels of 5 % and larger without damaging the wires. Since the used piezo-electric material, PMN-PT, is not capable of inducing strain levels above 0.5 %, damage to the wires is therefore not a great risk.

The large energy shifts that can be reached make it possible to tune any two nanowires into resonance, since the variation of emission energies between different wires does not exceed 10 meV. This is potentially interesting for applications which require single photon sources to spectrally overlap, for example to realize two-photon interference between two different nanowires.

### 7.4 Magneto-optical measurements

Using the setup described in Sec. 3.3, the NWQDs mounted on top of the piezoelectric actuator are exposed to magnetic fields up to 10 T. Contrary to the experiments presented in Ch. 5, the PL is both excited and collected perpendicular to the growth direction of the wires. Due to the orientation of the collection direction, the geometry of the measurement is not identical to the one used in Ch. 5. However, for the sake of simplicity, a magnetic field parallel or perpendicular to the NWQD growth direction will still be referred to as the Faraday and Voigt geometries respectively.

The measurements presented here aim to determine the electron and hole g-tensor. Assuming that the g-tensor is isotropic in-plane - an assumption which is fair since numerical calculations have shown only a small dependence on the azimuthal angle in InAs QDs [81] - the electron and hole g-tensor both consist out of two components ($g_x = g_y$ and $g_z$) for a total of four components. To resolve these components an additional measurement at an intermediate angle is required besides the Faraday and Voigt geometries. In this measurement, the sample is rotated in such a way that the magnetic field is applied under an angle of 30° with the nanowire growth axis. The choice for this angle was made for practical
reasons. The three configurations (Faraday, Voigt and intermediate) in which the experiment is performed are schematically shown in Fig. 7.6.

### 7.4.1 Poling-induced strain-shift

Due to the mounting of the wires on the piezo-electric substrate and cooling down of the device, a pre-strain will always be present in the QD on top of the built-in strain caused by the lattice mismatch between the QD and the wire. In between different measurements the poling direction was at one point reversed, which was found to have significant consequences for this pre-strain, shifting the emission energy of the wires up to 20 meV.

The experiment was performed in both the Faraday and the Voigt geometry before and after this re-poling event. Measurements before and after the event will be referred to as measurement 1 (M1) and measurement 2 (M2) respectively. The spectrum of wire A in the Voigt geometry measurements before and after the event is shown in Fig. 7.7. It is clear that the PL spectrum remains the same in the second measurement, however is red-shifted by 10.1 meV. This is true for the different excitonic complexes, which all exhibit the same shift when comparing M1 and M2.

Wires B, C and D show the same behaviour as wire A, where the spectrum in M2 is red-shifted compared to M1. However the magnitude of the red-shift varies a lot from wire to wire, being 3.1, 15.6 and 21.0 meV respectively. These large variations indicate that the observed red-shift is not likely to originate from the piezoelectric material itself; such large strain fluctuations over a relatively short range (the nanowires are separated by roughly 20 µm) are not to be expected. A physical change in the Platinum contacts with which the wires are fixed to the surface or possibly small fractures in the SiN layer created during the re-poling
Figure 7.7: Photoluminescence spectrum of wire A after (a) and before (b) reversing the poling direction, revealing a red-shift of 10.1 meV.

are more likely scenarios.

The signal-to-noise ratio for M1 is much worse (~50x) compared to M2, which can be seen in Fig. 7.7 and can most likely be attributed to differences in the alignment. This results in rather large experimental uncertainties in the determination of the g-factors $g_{exc}$ in M1, causing the strain-dependence of $g_{exc}$ to be undetectable within the range of uncertainty. For the measurements in M2, the strain-dependence could successfully be extracted.

Even though the sudden change in emission energy in between the different measurements is an unexpected and undesirable effect, it can actually be used as an advantage as it creates a point of reference for the determination of the strain-dependence of the exciton g-factor at an emission energy which would otherwise be out of range of the tunability of the device. The exciton g-factor determined in M1, without the strain-dependence, can then be used as an additional datapoint. The analysis in the subsequent sections will therefore be presented as follows: in the Faraday geometry the strain-dependence of the exciton g-factor obtained by varying the voltage across the piezoelectric actuator in M2 is compared with the strain-dependence of the exciton g-factor obtained from comparing M1 with M2 to show that the tunability of the exciton g-factor is valid over a wide range of emission energies. In the Voigt and intermediate geometries, only the data from M2 will be presented.

Apart from the large red-shift induced by inverting the poling directions,
measurement-to-measurement variations of the emission energy also occur on a much smaller scale. These variations are common in QD systems due to changes in the electronic environment [152] and can on top of that be caused by differences in the pre-strain after warming up the device and cooling it down again. In total five different measurements have been performed; in the Faraday and Voigt geometries in M1 and in the Faraday, Voigt and intermediate geometries in M2. A complete overview of emission energies (and their dependencies on the applied voltage) of the four different wires in the five different measurements is given in Table 7.1. For each wire only the emission energy of the charged exciton is given, as it is the most prominent complex and the other complexes show the exact same behaviour. The tunability of the emission energy with the applied voltage varies slightly from measurement to measurement. It varies a lot from wire to wire, which is likely to be caused by a different magnitude of the induced strain at a set voltage. It should be noted that the tunability of the emission energy achieved during the measurements here is roughly 4 times lower than it was in the characterization measurements in Sec. 7.4. This makes the maximum achieved strain \( \Delta \varepsilon_{zz} \approx 0.03\% \). The reason for this was not discovered.

### 7.4.2 Faraday geometry

Applying a magnetic field parallel to the nanowire growth direction is expected to yield a twofold splitting of the bright exciton state. Figure 7.8a, which shows the evolution of the PL spectrum for wire A with magnetic field, indeed shows each excitonic complex to split into two separate lines. Zooming in on each doublet shows the same behaviour for each of the three observed complexes. Each peak is fit with a Voigt profile. The choice for a Voigt profile is made empirically as
it visibly provides a better fit; using a Gaussian profile instead yields a slightly worse fit but the same results. The Zeeman splitting $\Delta E_{\text{Zeeman}}$ as a function of magnetic field is given by

$$\Delta E_{\text{Zeeman}} = \mu_B g_{\text{exc}} B$$ (7.1)

where $g_{\text{exc}} = g_{h,z} + g_{e,z}$ is the exciton g-factor. Looking at the Zeeman splitting as a function of magnetic field plotted in Fig. 7.8e reveals a smaller exciton g-factor (0.98 ± 0.01) for the charged exciton compared to the exciton and biexciton (1.04 ± 0.01), which are exactly equal to one another.

The strain-dependence of the exciton g-factor for wire A is finally shown in Fig. 7.8f, revealing the absolute value of the exciton g-factor to increase with increasing voltage and tensile strain. The increase appears linear, however the uncertainties are too large to exclude any non-linear contribution.

The measurement was repeated on the other three wires and the results are summarized in Table 7.2. The exciton g-factor shows rather large variations from wire to wire, roughly ranging from 1 to 1.7. This is not surprising since especially the out-of-plane hole g-factor is known to be sensitive to variations in size and composition of QDs [153, 25] and a similar magnitude of variations was observed for the self-assembled InGaAs QDs in Ch. 5.

The deviations of the exciton g-factor between the neutral and charged excitons, however small, fall outside of the error range and are consistent in the three wires (A, C and D) for which multiple lines were observed. In each case the charged exciton g-factor is a few percent smaller than the neutral exciton g-factor.
Figure 7.8: a) Full PL spectrum of wire A for various magnetic fields ranging from 0 T to 10 T applied in the Faraday geometry. Enlarged plots of the three visible peaks are shown in b), c) and d). e) Zeeman splitting of each line as a function of magnetic field, f) g-factor of the charged exciton as a function of the voltage applied to the piezoelectric actuator. The uncertainty range is indicated by the colored area.
A similar trend has been observed in self-assembled QDs [154], however conclusive evidence of its origin was not provided. In this case, the similarity between the exciton and biexciton $g$-factor and the difference between these two and the charged exciton $g$-factor exclude the influence of the Coulomb interaction as a possible cause, as this would also lead to differences between $X^0$ and XX. The exchange interaction is a more likely cause of the consistent difference in $g$-factors.

For each of the wires the tunability of the exciton $g$-factor is determined in the same way as illustrated for wire A in Fig. 7.8. Direct comparison of the wires with one another is not possible due to the large difference in tunability of the emission energy; each wire has a different magnitude of the induced strain at a set voltage. To properly compare the wires with one another, the tunability of the exciton $g$-factor with applied voltage is therefore divided by the tunability of the emission energy. This results in a change in $g$-factor per unit change in emission energy $dg/dE$. For each complex of each wire the exciton $g$-factor decreases with increasing emission energy, however the magnitude of the tunability varies between $-3 \text{ eV}^{-1}$ and $-6 \text{ eV}^{-1}$. No consistent difference between the charged exciton and neutral exciton is observed.

Finally the exciton $g$-factors for each wire before the re-poling event (M1) are listed in Table 7.3. By relating the difference in exciton $g$-factor between M1 and M2 to the difference in emission energy, $dg/dE$ is determined and compared with the results acquired in Table 7.2. This yields a good agreement, with most tunabilities falling within the range of uncertainty. This proves that the strain-

<table>
<thead>
<tr>
<th>Wire</th>
<th>Line</th>
<th>$E_{M1} - E_{M2}$ (meV)</th>
<th>$g$ (M1)</th>
<th>$g$ (M2)</th>
<th>$dg/dE$ (eV$^{-1}$)</th>
<th>$dg/dE$ (eV$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$X^*$</td>
<td>5.4</td>
<td>0.94</td>
<td>0.984</td>
<td>8 ± 1</td>
<td>2.9 ± 0.2</td>
</tr>
<tr>
<td></td>
<td>XX</td>
<td></td>
<td>1.00</td>
<td>1.045</td>
<td>8 ± 1</td>
<td>4 ± 1</td>
</tr>
<tr>
<td></td>
<td>$X^0$</td>
<td></td>
<td>1.00</td>
<td>1.044</td>
<td>8 ± 1</td>
<td>4.6 ± 0.2</td>
</tr>
<tr>
<td>B</td>
<td>$X^*$</td>
<td>3.1</td>
<td>1.18</td>
<td>1.203</td>
<td>7 ± 1</td>
<td>6.1 ± 0.2</td>
</tr>
<tr>
<td>C</td>
<td>$X^*$</td>
<td>15.6</td>
<td>1.22</td>
<td>1.270</td>
<td>4 ± 1</td>
<td>3 ± 1</td>
</tr>
<tr>
<td></td>
<td>$X^0$</td>
<td></td>
<td>1.33</td>
<td>1.383</td>
<td>5 ± 1</td>
<td>5 ± 1</td>
</tr>
<tr>
<td>D</td>
<td>$X^*$</td>
<td>21</td>
<td>1.52</td>
<td>1.633</td>
<td>5 ± 1</td>
<td>-6.6 ± 0.6</td>
</tr>
<tr>
<td></td>
<td>XX</td>
<td></td>
<td>1.61</td>
<td>1.734</td>
<td>6 ± 1</td>
<td>6 ± 3</td>
</tr>
<tr>
<td></td>
<td>$X^0$</td>
<td></td>
<td>1.62</td>
<td>1.732</td>
<td>5 ± 1</td>
<td>4.3 ± 0.6</td>
</tr>
</tbody>
</table>

Table 7.3: Comparison of the $g$-factor between the two different measurements M1 and M2 for each line and wire. The acquired tunability of the $g$-factor with emission energy is compared to the one previously acquired in Table 7.2.
dependent measurement can be used as a probe to determine the tunability of the g-factor over a wider range.

### 7.4.3 Voigt geometry

Applying a magnetic field perpendicular to the nanowire growth direction yields a fourfold splitting of the excitonic complexes, as is shown in Fig. 7.9. However, unlike the Faraday geometry, there are significant differences between the different excitonic complexes. For the $X^*$ complex, all four lines are already visible at low magnetic fields, becoming fully distinguishable at a magnetic field strength of 3T. The Zeeman splitting between the outermost peaks and the Zeeman splitting between the innermost peaks are each characterized by their own g-factor, which will be referred to as $g_1$ (outer peaks) and $g_2$ (inner peaks) respectively. These g-factors are defined by either the sum of or the difference between the in-plane electron and hole g-factors, however it is not yet known in what order. The observation that the difference between $g_1$ and $g_2$ is relatively small therefore indicates a near-zero electron or hole g-factor.

The neutral excitonic complexes $X^0$ and XX exhibit a different behaviour; rather than all four lines being present at low magnetic fields, two of the lines are revealed only at higher magnetic fields. The intensity of these lines increases significantly with magnetic field.

Inspection of the eigenstates as given in Ref. [66] immediately shows that at zero magnetic field the two higher energy states are the bright excitons, while the two lower energy states are the dark excitons. A non-zero magnetic field applied in the plane of the quantum dot breaks its symmetry, leading to a mixing between the bright and dark states, causing also the dark states to become visible. However, only when the Zeeman splitting is of the same order of magnitude as the exchange splitting this mixing becomes significant. With increasing magnetic field, the mixing between the bright and dark states increases, hence the intensity of the dark emission also increases. This explains why for the exciton two peaks (the dark excitons) appear on the low energy side at higher magnetic fields. This is not the case for the charged exciton, since due to the absence of exchange interaction the bright and dark excitons are already fully mixed at low magnetic fields.

For the biexciton the situation is reversed compared to the neutral exciton; the dark excitons appear on the high energy side instead. This can easily be explained by considering the biexciton recombination scheme in Fig. 7.10, which shows that while for the exciton the bright emission is on the high energy side of the dark emission, the situation is reversed for the biexciton. This is due to the simple fact that the total energy of the biexciton cascade $E_{XX}$, which is the
Figure 7.9: a) Full PL spectrum of wire A for various magnetic fields ranging from 0 T to 10 T applied in the Voigt geometry. Enlarged plots of the three visible peaks are shown in b), c) and d). The corresponding Zeeman splittings are shown in e), f) and g) and fit with Eq. 7.2, revealing the expected linear behaviour for $X^*$ and non-linear behaviour for the $X^0$ and $XX$. 

Counts (a.u.)
Energy (eV)


Zeeman splitting (meV)
Magnetic Field (T)
0 2 4 6 8 10

Counts (a.u.)
Energy (eV)

1.283 1.2834 1.2838
1.2872 1.2876 1.288
1.2888 1.2892 1.2896

Energy (eV)

0 2 4 6 8 10
Magnetic Field (T)

Zeeman splitting (meV)
Magnetic Field (T)
0 2 4 6 8 10
sum of the biexciton to exciton transmission \( E_{XX \rightarrow X^0} \) and the exciton to zero transmission \( E_{X^0 \rightarrow 0} \) is the same for the bright and dark states. Therefore if \( E_{X^0 \rightarrow 0, bright} > E_{X^0 \rightarrow 0, dark} \) then \( E_{XX \rightarrow X^0, bright} < E_{XX \rightarrow X^0, dark} \).

In Fig. 7.9c and 7.9d it is clear that extrapolating the Zeeman-split quadruplet to a magnetic field of 0 T results in a splitting between the bright and dark states at zero magnetic field. This is related to the exchange interaction and can be quantified by considering the emission energies of the four transitions as a function of magnetic field, which are given in Eq. 2.41. The two Zeeman splittings, \( \Delta E_1 = E_1 - E_4 \) and \( \Delta E_2 = E_2 - E_3 \) are given by

\[
\Delta E_1 = \frac{1}{2}\sqrt{(2\delta_0 + \delta_1 - \delta_2)^2 + 4\mu_B^2(g_{e,x} - g_{h,x})^2B^2},
\]

\[
\Delta E_2 = \frac{1}{2}\sqrt{(2\delta_0 - \delta_1 + \delta_2)^2 + 4\mu_B^2(g_{e,x} + g_{h,x})^2B^2}.
\]

At zero magnetic field, the two sets of peaks are already split by

\[
\Delta E_{1,B=0} = |\delta_0 - \frac{1}{2}(\delta_2 - \delta_1)|,
\]

\[
\Delta E_{2,B=0} = |\delta_0 + \frac{1}{2}(\delta_2 - \delta_1)|,
\]

which explains why this zero-field splitting is observed for \( X^0 \) and \( XX \), but not for \( X^* \). When neglecting the exchange splitting, which is justified for the charged exciton or in the limit of high magnetic field, the Zeeman splittings reduce to \( \mu_B(g_{e,x} \pm g_{e,h})B \).

The experimentally obtained Zeeman splittings shown in Figs. 7.9e, 7.9f and 7.9g indeed show the expected behaviour; linear for the charged exciton and non-
linear at low magnetic fields for the neutral exciton and the biexciton. The data is fit with Eqs. 7.2, including the exchange terms for $X^0$ and $XX$, but removing them for $X^*$. 

For $X^0$ and $XX$ these fits give information about the magnitude of the exchange interaction. For the neutral exciton the outer two peaks are split by $252 \pm 4 \mu eV$ at zero magnetic field, while the inner two peaks are split by $240 \pm 3 \mu eV$. This agrees well with the biexciton, where the two sets of peaks are split by $257 \pm 8 \mu eV$ and $242 \pm 17 \mu eV$. Since the zero-field splittings of the two sets of peaks are comparable, the bright and dark FSS $\delta_1$ and $\delta_2$ must also have a comparable magnitude. In none of the measurements a fine structure splitting of the exciton has been observed within the experimental accuracy ($<30 \mu eV$). A vanishing fine structure splitting of the bright exciton was predicted for WZ nanostructures [155], and values of $\delta_1 = 4 \mu eV$ [156] and $\delta_1 = 8 \mu eV$ [147] have been reported for comparable InAsP NWQDs. The notion that the bright FSS $\delta_1$ is small then implies the same for the dark FSS $\delta_2$, while the electron-hole exchange energy has a sizable value of $\delta_0 = 246 \pm 4 \mu eV$ for the exciton. This agrees well with the work of Witek et al. [156], where values of 164, 18 and 4 $\mu eV$ were extracted for $\delta_0$, $\delta_1$ and $\delta_2$ respectively in a similar InAsP NWQD system.

**Strain-dependence**

Analogous to the Faraday geometry, the Zeeman splitting can now be determined as a function of the voltage applied to the piezoelectric actuator. Due to their non-linear behavior, the exciton and biexciton require more data points to accurately determine their g-factors compared to the charged exciton, where the Zeeman splitting has a purely linear dependence on magnetic field due to the absence of the exchange interaction. In the Faraday geometry no significant difference was found in the exciton g-factor and its strain-dependence between the charged and neutral excitons. Therefore it is sufficient to analyze only the charged exciton $X^*$. 

The results for wire A are shown in Fig. 7.11. Both the g-factors decrease when applying tensile strain to the system. The outer peaks are affected more than the inner peaks, with slopes of $(-0.7 \pm 1)10^{-5}V^{-1}$ and $(-0.4 \pm 0.1)10^{-5}V^{-1}$ respectively. The results for all wires are shown in Table 7.4.

For each wire, both g-factors show the same trend in each case; a decrease with increasing tensile strain. However, the magnitude of this decrease varies.

**Other wires**

The same analysis was performed on the other three wires. For each of these wires, the PL spectrum at a magnetic field strength of 10 T is shown in Fig. 7.12.
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

Figure 7.11: Exciton g-factors for the charged exciton as a function of the voltage applied to the device. Both exhibit a decrease in absolute sense.

<table>
<thead>
<tr>
<th>Wire</th>
<th>$g_1$</th>
<th>$g_2$</th>
<th>$dg_1/dV$</th>
<th>$dg_2/dV$</th>
<th>$dg_2/dE$</th>
<th>$dg_2/dE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.159</td>
<td>0.865</td>
<td>-0.7 ± 0.1</td>
<td>-0.4 ± 0.1</td>
<td>1.3 ± 0.2</td>
<td>0.7 ± 0.2</td>
</tr>
<tr>
<td>C</td>
<td>1.094</td>
<td>0.918</td>
<td>-0.4 ± 0.2</td>
<td>0.0 ± 0.1</td>
<td>2 ± 1</td>
<td>0 ± 1</td>
</tr>
<tr>
<td>D</td>
<td>1.054</td>
<td>0.884</td>
<td>-0.4 ± 0.2</td>
<td>-0.2 ± 0.2</td>
<td>1.1 ± 0.5</td>
<td>0.5 ± 0.5</td>
</tr>
</tbody>
</table>

Table 7.4: Emission energy, $g$-factors and their tunabilities for the charged exciton of wires A, C and D with the magnetic field applied perpendicular to the NWQD growth direction. In the last column the tunability of the $g$-factors with emission energy is given.

However, for wire B the four peaks could not be fully resolved. Instead, a small shoulder is observed on the outside of each of the two main peaks, implying that either the electron or hole $g$-factor is close to zero. This makes the analysis for this wire impossible.

Wire C behaves as expected and the four peaks are easily resolved at 10 T. For wire D only three peaks are observed, rather than four. It appears that one of the lines is simply missing on the right-hand side of the spectrum. When moving the laser spot across the wire, the second peak on the right-hand side does become visible, while one of the peaks on the left-hand side disappears. This behaviour is completely unexpected and the reason for this was not discovered. The observation that the visibility of the peaks depends on the exact spot on the wire where the PL is collected from could indicate some directionality of the PL emission. However, if this directionality would be caused by for example the polarization of the peaks, always two peaks would be missing instead of one, which is clearly not the case. Fortunately, since the splitting of the charged exciton is symmetric, the $g$-factors
Figure 7.12: Spectrum of the charged exciton of wires B, C and D at a magnetic field of 10 T. For wire B the splitting is too small to resolve the four different peaks. Wire C behaves as expected, while wire D is missing one of the peaks.

can still be determined for wire D.

7.4.4 Intermediate measurement

To be able to determine both the in-plane and out-of-plane components of the g-tensor for the electron and hole separately, an intermediate measurement is required. In this measurement, the sample is rotated in such a way that the magnetic field is applied under an angle of 30° with the nanowire growth axis.

The PL spectrum of wire A as a function of magnetic field is shown in Fig. 7.13a, where it is split up into $X^*$, $XX$ and $X^0$ in Figs. 7.13b, 7.13c and 7.13d. As for the Voigt geometry, it is clear that the charged exciton splits up symmetrically into four lines. The neutral exciton and biexciton on the other hand show a strong asymmetry and are mirror images of each other.

The Zeeman splittings as a function of magnetic field are depicted in Figs. 7.13e, 7.13f and 7.13g. Again similar to the Voigt geometry, the charged exciton shows the expected linear behaviour, while the neutral exciton and biexciton are strongly non-linear at low magnetic fields. The strain-dependence of the g-factors in the intermediate geometry is shown in Fig. 7.14. Results for the other wires are summarized in Table 7.5.

7.5 Resolving the full g-tensor

With the experiment performed in all three geometries (Faraday, Voigt and intermediate), the full g-tensor for the electron and hole can be determined separately. The strain-independent case for wire A is discussed first. There are four indepen-
Figure 7.13: a) Full PL spectrum of wire A for various magnetic fields ranging from 0 T to 10 T applied in the intermediate geometry. Enlarged plots of the three visible peaks are shown in b), c) and d). The corresponding Zeeman splittings are shown in e), f) and g), revealing the expected linear behaviour for $X^*$ and non-linear behaviour for the $X^0$ and $XX$. 

Zeeman splitting (meV) vs Magnetic field (T)
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

Figure 7.14: g-factors for the charged exciton as a function of the voltage applied to the device.

<table>
<thead>
<tr>
<th>Wire</th>
<th>$g_1$</th>
<th>$g_2$</th>
<th>$dg_1/dV$</th>
<th>$dg_2/dV$</th>
<th>$dg_2/dE$</th>
<th>$dg_2/dE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.049</td>
<td>0.861</td>
<td>1 ± 0.1</td>
<td>-1.5 ± 0.1</td>
<td>-1.7 ± 0.2</td>
<td>2.6 ± 0.2</td>
</tr>
<tr>
<td>C</td>
<td>1.246</td>
<td>0.636</td>
<td>0.6 ± 0.1</td>
<td>-0.6 ± 0.3</td>
<td>-3.2 ± 0.5</td>
<td>3.2 ± 0.5</td>
</tr>
<tr>
<td>D</td>
<td>1.620</td>
<td>0.217</td>
<td>2.5 ± 0.2</td>
<td>-2.9 ± 0.4</td>
<td>-6 ± 1</td>
<td>7 ± 1</td>
</tr>
</tbody>
</table>

Table 7.5: Emission energy, g-factors and their tunabilities for the charged exciton of wires A, C and D with the magnetic field applied under an angle of 30° with the NWQD growth direction. In the last column the tunability of the g-factors with emission energy is given.

dent components of the g-tensor to be determined; in-plane and out-of-plane for the electron and hole, which have to satisfy the following conditions related to the g-factors observed in the experiments:

\[

g_F = g_{h,z} + g_{e,z},
\]

\[
g_{V1} = g_{h,x} \pm g_{e,x},
\]

\[
g_{V2} = g_{h,z} \mp g_{e,x},
\]

\[
g_{I1} = \sqrt{\frac{1}{4}g_{e,x}^2 + \frac{3}{4}g_{e,z}^2 + \sqrt{\frac{1}{4}g_{h,x}^2 + \frac{3}{4}g_{h,z}^2}},
\]

\[
g_{I2} = \pm \left(\sqrt{\frac{1}{4}g_{e,x}^2 + \frac{3}{4}g_{e,z}^2} - \sqrt{\frac{1}{4}g_{h,x}^2 + \frac{3}{4}g_{h,z}^2}\right).
\]

Fitting the g-factors shown in Tables 7.2, 7.4 and 7.5 to this set of equations defines the values of the g-tensor components, but does not yet unambiguously determine their signs. It was previously mentioned that in-plane either the electron or hole g-factor is close to zero; analogous to the self-assembled quantum dots presented in Ch. 5 it is assumed that this is the hole g-factor. This leads to $g_{e,z} = \pm 0.931$, $g_{h,z} = \pm 0.058$, $g_{e,x} = \pm 1.013$, $g_{h,x} = \pm 0.149$, where $g_{e,z}$ and $g_{h,z}$ carry the same
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

Figure 7.15: Out-of-plane and in-plane components of the electron and hole g-tensors. The out-of-plane hole g-tensor is found to be most strongly dependent on the applied strain.

In Ch. 6 the electron g-factors were calculated to be $g_{e,z} = 1.21$ and $g_{e,x} = 1.27$. Since these values agree well with those that follow from the experiment and the small anisotropy between $g_{e,z}$ and $g_{e,x}$ is well reproduced, it is inferred that both are positive. The sign of $g_{h,z}$ is then positive as well. The sign of $g_{h,x}$ cannot be determined and it is not essential to do so.

Looking back at Table 7.1, the sensitivity of the emission energy to the applied voltage is slightly different for each of the three measurements. This implies that at a set voltage, the amount of stress the system is exposed to is also slightly different for each measurement. However, since these differences are relatively small ($\approx 10\%$), this can be disregarded and the strain-dependence of the components of the g-tensors can be determined by performing the fitting procedure described in the previous paragraph to the three measurements at each set voltage.

The final result for the strain dependence of $g_{e,z}$, $g_{e,x}$, $g_{h,z}$ and $g_{h,x}$ is shown in Fig. 7.15. For clarity each y-axis is chosen to cover an equal range. This makes it immediately clear that the out-of-plane hole g-factor is by far most sensitive to the applied strain, both in absolute and in relative sense. Because in this case coincidentally the hole g-factor has a value close to zero, the change is as large as 20 %. The other components show a much smaller sensitivity, where especially the in-plane hole g-factor is more or less completely unaffected.

These results, as well as for the other wires, are summarized in Table 7.6. The electron and hole will now be discussed separately.
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

Table 7.6: g-factors and their sensitivities as a function of voltage applied to the piezoelectric actuator and change in emission energy. In the bottom row results from the calculations in Ch. 4 are given.

<table>
<thead>
<tr>
<th>Wire</th>
<th>$g_{h,z}$</th>
<th>$g_{h,x}$</th>
<th>$g_{e,z}$</th>
<th>$g_{e,x}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.058</td>
<td>0.149</td>
<td>0.931</td>
<td>1.013</td>
</tr>
<tr>
<td>C</td>
<td>0.358</td>
<td>0.088</td>
<td>0.918</td>
<td>1.010</td>
</tr>
<tr>
<td>D</td>
<td>0.789</td>
<td>0.086</td>
<td>0.872</td>
<td>0.975</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wire</th>
<th>$dg_{h,z}/dV$</th>
<th>$dg_{h,x}/dV$</th>
<th>$dg_{e,z}/dV$</th>
<th>$dg_{e,x}/dV$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$10^{-5}$</td>
<td>-0.4 ± 0.1</td>
<td>-0.1 ± 0.1</td>
<td>-0.5 ± 0.1</td>
</tr>
<tr>
<td>C</td>
<td>0.7 ± 0.2</td>
<td>-0.1 ± 0.1</td>
<td>-0.1 ± 0.2</td>
<td>-0.1 ± 0.1</td>
</tr>
<tr>
<td>D</td>
<td>2.9 ± 0.3</td>
<td>-0.1 ± 0.3</td>
<td>-0.4 ± 0.3</td>
<td>-0.2 ± 0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wire</th>
<th>$dg_{h,z}/dE$</th>
<th>$dg_{h,x}/dE$</th>
<th>$dg_{e,z}/dE$</th>
<th>$dg_{e,x}/dE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-4.2 ± 0.2</td>
<td>0.2 ± 0.2</td>
<td>0.7 ± 0.2</td>
<td>0.9 ± 0.2</td>
</tr>
<tr>
<td>C</td>
<td>-4 ± 1</td>
<td>1 ± 1</td>
<td>1 ± 2</td>
<td>1 ± 1</td>
</tr>
<tr>
<td>D</td>
<td>-8 ± 1</td>
<td>0 ± 1</td>
<td>1 ± 1</td>
<td>1 ± 1</td>
</tr>
</tbody>
</table>

| Calculations | -9.52 | 0 | 1.31 | 0.61 |

**Electron g-factor**

The three NWQDs have nearly identical values for the in-plane and out-of-plane electron g-factors, in terms of both value and sensitivity. For each dot, $g_x$ has a value around 1 and is slightly larger than $g_z$, which has a value of around 0.9. This agrees well with the anisotropy calculated Ch. 6, where values of $g_x = 1.27$ and $g_z = 1.21$ were found. Both the electron g-factors decrease as a function of tensile strain, however the sensitivities are low at roughly 1 eV$^{-1}$. This is significantly lower than the 5 eV$^{-1}$ which was found for $g_x$ in the self-assembled QDs in Ch. 5, where the sensitivity of the electron g-factor was ascribed to the effect of strain on the confinement and consequently the lateral extension of the electron wavefunction. The calculations in Ch. 6 have shown that the effect of strain on the confinement in the WZ NWQDs used for the experiments here is negligible. Instead, the electron g-factor is affected only by the strain-dependence of the band edges, which change the contributions of each of the valence bands to the electron g-factor and result in a small net decrease with tensile strain. In the calculations sensitivities of 1.3 and 0.6 eV$^{-1}$ were found for $g_z$ and $g_x$ respectively, agreeing well with the experimental results presented here.
Hole g-factor

For each of the three wires \( g_{h,x} \) is close to zero and insensitive to strain within the experimental accuracy. In WZ materials the heavy hole and light hole bands are split up even in bulk. In a NWQD the strain introduced by the lattice mismatch between the dot material and the host material splits these bands up even further. The hole ground state wavefunction is therefore strongly dominated by the heavy hole. Analogous to the self-assembled QDs in Ch. 5, because the heavy hole has an in-plane g-factor of zero, a close-to-zero and strain-insensitive in-plane hole g-factor is therefore to be expected.

The only g-tensor component which varies from dot to dot is the out-of-plane hole g-factor \( g_{h,z} \), ranging from 0.06 in wire A to 0.79 in wire D. This wide variation is not unusual, as the hole g-factor is known to be extremely sensitive to the exact size, shape, composition and built-in strain of the QD [25, 28]. As a consequence \( g_{h,z} \) is also more sensitive to strain than any of the other components. High sensitivity of \( g_{h,z} \) was also observed for the self-assembled QDs in Ch. 5. In both systems the splitting between the heavy hole band and the light hole band increases with increasing strain, resulting in an increase of \( g_{h,z} \). This was shown in Ch. 6, where a sensitivity of \(-9.5 \ \text{eV}^{-1}\) for \( g_{h,z} \) was calculated. The agreement with the experimental results presented here, where sensitivities ranging from -4 to -8 eV\(^{-1}\) are found, is reasonable.

7.6 Conclusions

In this chapter a piezoelectric actuator was used to apply uniaxial strain to nanowire quantum dots. The fabricated device is capable of inducing strains of up to at least \( \Delta \epsilon_{zz} = 0.3\% \), corresponding to a shift of the emission energy of 20 meV. The device was used to investigate the strain-dependence of the electron and hole g-tensors. In the magneto-luminescence experiments performed to do so the induced strain was limited to \( \Delta \epsilon_{zz} = 0.03\% \), but this proved to be sufficient to extract the strain-dependence of all four g-tensor components, which was done by performing the experiment in three different geometries; in the Faraday geometry, Voigt geometry and an intermediate geometry where the magnetic field was applied under an angle of 30° with the NWQD growth axis. In the Faraday geometry a consistent difference between the g-factor of the neutral excitons (X\(^0\) and XX) and the charged exciton (X\(^+\)) was found, hinting at the role of the exchange interaction. The experiment in the Voigt geometry revealed that the bright and dark fine structure splittings are negligible within the experimental accuracy. The electron-hole exchange interaction was found to be significant with \( \delta_0 = 246 \pm 4 \ \mu \text{eV} \).
Chapter 7. Magneto-optical characterization of a strained nanowire quantum dot

The determination of the electron and hole g-tensors focused on the charge exciton, as the exchange interaction then doesn’t have to be taken into account and the measurement in the Faraday geometry revealed no significant differences in the strain-dependence of the exciton g-factor between the different excitonic complexes. The three wires which have been fully investigated all showed a small anisotropy between the in-plane and out-of-plane electron g-factors, with \( g_{e,x} \approx 1 \) and \( g_{e,z} \approx 0.9 \). This anisotropy was well reproduced by the calculations presented in Ch. 6. The observed strain-sensitivity of both components of \( \approx 1 \text{ eV}^{-1} \) also agreed well with the calculations. The calculations showed that, contrary to the self-assembled QDs in Chs. 4 and 5, the confinement energy of the electron does not play a role in the strain-sensitivity of the electron g-factors. Instead, the observed sensitivity is purely caused by changes in the band edge energies with strain, affecting the contributions of each of the valence bands to the electron g-factors.

The in-plane hole g-factor \( g_{h,x} \) was found to be close to zero and insensitive to strain, which was explained by considering the strong heavy hole character of the hole ground state. Similar to the self-assembled QDs in Chs. 4 and 5, the out-of-plane hole g-factor \( g_{h,z} \) showed the largest sensitivity to induced strain, which is due to the effect of strain on the separation between the different valence bands.

To achieve tunability of one of the g-tensor components around zero, \( g_{h,z} \) is the most suitable candidate. Using the full potential of the device, strains up to \( \Delta \epsilon_{zz} = 0.3 \% \) can be applied, leading to changes in \( g_{h,z} \) of 0.1-0.2. This can be further enhanced by adjusting the QD parameters. For example, increasing the sensitivity of the confining potential to strain will consequently increase the sensitivity of \( g_{h,z} \).
Summary

Active manipulation of the g-tensor in semiconductor nanostructures

Semiconductor quantum dots (QDs) are promising candidates for future quantum technologies, as they can be exploited as sources of single photons or hosts of quantum bits. Besides charge, electrons and holes also carry a spin, which can be used to store and process information. The spin of an electron can be manipulated by controlling an externally applied magnetic field. This approach proves challenging to scale up, as it is difficult to locally apply magnetic fields on a QD scale. Another approach is to gain control over the interaction of the electron with the magnetic field, rather than the magnetic field itself. This interaction is governed by the g-tensor, which in QDs is generally anisotropic due to the confining potential. By tuning one of the components of the g-tensor, which are referred to as g-factors, full control over the spin of an electron or hole can be achieved. This requires a way to in-situ manipulate the electronic structure of a QD, which in this thesis is realised by means of externally induced strain. Two different systems based on two different crystal structures, Wurtzite and Zinc Blende, are investigated through experiments as well as calculations.

In Ch. 4 an eight-band $k\cdot p$-model is employed to investigate the influence of biaxial compressive strain on the electron and hole g-tensors of an InGaAs/GaAs QD. The main contributions of this biaxial compressive strain to the band structure are an increase in the band gap and an increase in the splitting between the heavy hole and light hole bands, which has consequences for the electron and hole g-tensors. For the electron g-tensor both the in-plane and out-of-plane components are discovered to experience a small increase with the induced strain, which is explained by considering the large penetration of the electron ground state wavefunction into the barrier due to the shallow confinement in the conduction band. Roughly half of the probability density is found to be outside the QD. Biaxial compressive strain results in a relatively large increase of the barrier height which increases the quenching of the orbital momentum and therewith the electron g-factors. The anisotropy of the confining potential accounts for the observed larger sensitivity of the in-plane electron g-factor compared to its out-of-plane counterpart, as it quenches the orbital contribution to the electron g-factor more in one direction that in the other. A large anisotropy is found for the hole g-tensor, where the sensitivity of the in-plane component is negligible and the out-of-plane...
component is found to be extremely sensitive to strain. The close-to-zero value and the negligible strain-dependence of the in-plane hole g-factor is explained by considering the strong heavy hole-like character of the hole ground state wavefunction, since a pure heavy hole state has a zero in-plane g-factor. The remarkable sensitivity of the out-of-plane hole g-factor is ascribed to the effect of the strain-dependent heavy hole-light hole splitting on the composition of the hole ground state wavefunction.

The experimental realization of these numerical calculations is presented in Ch. 5, where biaxial compressive strain is incorporated in thin nanomembranes containing self-assembled InGaAs/GaAs QDs by means of a piezoelectric actuator. By performing magneto-optical measurements in different orientations of the applied magnetic field the electron and hole g-tensors are extracted separately. The strain-dependence of the electron and hole g-tensors is investigated for five different QDs, showing consistent results. An excellent agreement is established for all components of the electron and hole g-tensors between the experimental results and the numerical calculations, both qualitatively and quantitatively. These results suggest that the out-of-plane hole is the most suitable candidate for spin manipulation via g-tensor modulation, especially when engineering the size, shape and composition of QDs to bring the value of the out-of-plane hole g-factor closer to zero. The in-plane electron g-factor also remains a suitable candidate, as its strong dependence on confinement can be exploited in shallow QDs.

In Chs. 4 and 5 the strain-dependence of the exciton diamagnetic coefficient is investigated as well, as it is a direct probe of the lateral extension of the exciton wavefunction. The numerical calculations reveal that the contribution of the hole to the exciton diamagnetic shift is negligible. The experimentally determined exciton diamagnetic coefficient is then dominated by the electron. The observed decrease of the electron diamagnetic coefficient with strain for magnetic fields applied both parallel and perpendicular to the QD growth direction is directly linked to the lateral extension of the electron by calculating the spread of the probability density in all directions. The same dependence is found in the experiment, verifying the previous notion that the electron g-factors increase due to a decrease of the lateral extension of the electron wavefunction. From the surprisingly large sensitivity of the diamagnetic coefficients it is deducted that in these experiments the diamagnetic shift can be used to probe changes in the lateral extension of the electron wavefunction with sub-angstrom precision.

Inspired by the promising results obtained on the Zinc Blende self-assembled QDs, the second part of this thesis focusses on a different material system, Wurtzite InAsP nanowire quantum dots. The reduced volume of nanowires compared to the
nanomembranes used with the self-assembled quantum dots makes them suitable to apply higher amounts of strain. Furthermore, in III-V nanowires one often encounters the Wurtzite crystal structure (WZ) rather than the Zinc Blende (ZB) crystal structure. The anisotropy of the WZ crystal leads to new effects such as an anisotropy in the spin-orbit interaction. The ability to grow nanostructures in the WZ structure is relatively new and therefore many aspects have not yet been thoroughly investigated.

In an attempt to contribute to the expanding pool of knowledge about WZ III-V systems, in Ch. 6 a primitive model is presented to calculate the electron g-factors in WZ bulk materials and nanostructures. In ZB materials anisotropy of the electron g-tensor is only obtained when introducing an anisotropic confining potential. In WZ materials this anisotropy is present even in bulk due to the hexagonal crystal structure. For InP the anisotropy of the electron g-tensor is defined by the anisotropy of the Kane energy, while for InAs the opposite anisotropy is found. The Kane energies for WZ are generally smaller than those for ZB, leading to higher values of the electron g-factors in WZ materials. Experimental data is limited, however the in-plane electron g-factor calculated for InP agrees well with reported values. It would be worthwhile to experimentally disentangle the electron and hole g-tensors in bulk WZ InAs and InP to properly test these findings and obtain reliable values for the momentum matrix elements.

By modifying energy differences in the expressions for the electron g-factors with quantization energies calculated using a one-band effective mass approximation, the electron g-factors for an InAsP NWQD are calculated. The introduction of this effective band gap affects the in-plane electron g-factor more than it does the out-of-plane component and the anisotropy of the electron g-tensor reverses compared to bulk. Using the strain distribution in the InAsP NWQD, which is calculated using a finite element method, the strain-dependence of the electron g-tensor is investigated. The electron g-factors are only affected by strain due to a modification of the band edge energies, which affects the contributions of the various valence bands to the electron g-factors. This is fundamentally different from the electron g-tensor for the ZB self-assembled QDs, where the strain-dependence is dominated by a change in the confining potential with strain. The strain-dependence of the out-of-plane hole g-factor is estimated by using a known expression for bulk WZ materials, leading to a one order of magnitude higher sensitivity compared to the electron g-factors.

By fixing a nanowire containing a quantum dot across a gap etched in a piezoelectric actuator, homogeneous uniaxial strain is applied to NWQDs in Ch. 7. This makes it possible to induce shifts of the QD emission energy up to 20 meV.
The electron and hole g-tensors are obtained by performing magneto-luminescence experiments in different orientations of the external magnetic field. The resulting values for the electron g-factors correspond well with those calculated in Ch. 6 and the same anisotropy is obtained. The observed decrease of both the in-plane and out-of-plane electron g-factor is also quantitatively supported by the calculations. The hole g-tensor has a strain-insensitive in-plane component which is close to zero, and a strongly strain-sensitive out-of-plane component. The sensitivity of the out-of-plane hole g-factor exceeds the sensitivity of the electron g-factors by one order of magnitude and is well reproduced by the calculations.

The experiments and calculations presented in this thesis demonstrate that strain can be employed as a powerful tool to affect the electronic structure in semiconductor QDs. The out-of-plane hole g-factor is designated as the most promising candidate to achieve tunability around zero. The role of the splitting between the different valence bands is crucial. This knowledge can be exploited to obtain even larger tunabilities by maximizing the effect of strain on the mixing between the heavy and light hole bands, for example in a strain-free system such as AlGaAs/GaAs QDs. Large tunabilities of the electron g-factors can be obtained in shallow QDs where strain has a large influence on the barrier height. Through the use of new micromachining techniques strain-control of nanostructures can be incorporated in microscopic devices, which opens the door to a new way of controlling spins at a single QD scale.
Acknowledgements

There are many people who have contributed to this thesis in one way or another, both professionally and personally. I could mention everyone explicitly and say something about all of them, but the risk of forgetting someone is simply too big. Besides, that would most likely double the size of this thesis. I would therefore like to simply summarize by thanking my colleagues, my friends, my family and everyone I went to a concert or pub quiz with, or played a board game with, or generally spent a pleasant day or evening with, for their support and/or company in the past years. In principle I could end these acknowledgements here, however there are of course some people (warning: some means actually quite a lot) who deserve a special mention.

Paul and Andrei, thank you for giving me the opportunity to complete this work within your group, and for giving me a push in the right direction whenever I needed it. Without your guidance, advice and discussions this thesis would not have existed. Paul, I admire your enthusiasm for nearly anything, whether we are discussing physics or something completely unrelated. Andrei, you are like a walking encyclopedia. In the rare occasion that you did not know the solution to a question or problem I posed, you would at least know a few references where to find it. No matter what topic, you always have a story to go with it, which has contributed to many interesting coffee and lunch breaks.

Special thanks also go to my second promotor, Armando. I have enjoyed our fruitful and pleasant collaboration, which has led to two publications. It was a great pleasure to visit your group in the very beginning of my PhD. Without the samples made by your group (for which I also thank Rinaldo and Johannes), two of the chapters in this thesis would have been non-existent.

When it comes to the modelling part of my PhD, Craig was indispensable. My Master internship with you was my first real introduction into theoretical work (and Python), which later formed a solid basis for my PhD. During my PhD you advised me countless times and were always happy to help. Thank you for the pleasant and always helpful discussions.

Dan, your nanowires were crucial to the second part of my PhD. You spent a lot of time optimizing the growth process for our needs, resulting in the beautiful
NWQDs that we have used extensively. Without you the last chapter of this thesis would not have been possible.

The time-gated nature of a PhD has an interesting consequence; the colleagues that are present when you start your PhD are all gone by the time you finish. The beginning of my PhD was mainly characterized by a large number of Italians, after-Borrel dinners and evenings at Alessandros place. Thanks to everyone who welcomed me into the group in my early days.

After I started my PhD, the number of Italian colleagues slowly started to decrease. Coincidentally, this was accompanied by a decrease in the amount of yelling during our football matches. I know from first-hand experience how dangerous playing football can be, however I have always enjoyed being part of the football team. Our team spirit was definitely unbreakable. Thanks to everyone who has been part of the Leaky Labs (previously PSN) team over the years.

During the second half of my PhD I spent a lot of time with part of the Dutch community within our group; Kaylee, Sander, Douwe, Rianne and Anne (yes Anne, you count as Dutch now). Whether it is a pub quiz (sometimes with Bas), board game night or barbecue (sometimes with Roeland), I have always enjoyed your company and look forward to our future adventures.

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One of the perks of doing a PhD is that occasionally you get to go to a con-
fERENCE in (usually) an interesting country, meeting fellow physicists from all over
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between The Netherlands and Germany, and most importantly, cake.

There are many people outside of my work life who have been important to me
during my PhD, or my life in general. One group that would definitely compete
for the prize of best group of friends in the Netherlands (if such a prize existed,
and I believe it should), is my group of high school "Sondervick" friends (Bertina,
Gregory, Heleen, Jorn, Jurriën, Kevin, Maarten, Patrick, Peter, Ted and of course
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Our yearly getaway is generally one of the highlights of the year.

Another yearly highlight is my summer camp, of which I have now been part
for more than ten years. It is nice to escape from reality once a year and organize
this great week, with great people, for great people. Besides that, it has resulted
in some dear friendships. Peter, besides my cousin you are also a great friend.
Stijn and Meike, you are always therefore me, even when I don’t need it, and
I can discuss anything with you. Special mention goes to Bastiaan and to Kim-
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Few people know that I have long been a member of one of the greatest bands in
the world. Kevin, Stefan and Rianne, although we dismissed our (fake) guitars
years ago, I always enjoy our time together. Kevin, you have been one of my
best friends for a very long time. Together we invent the greatest gimmicks and
we often end up having even more fun creating them than actually executing them.

De laatste woorden zijn ingericht voor mijn familie. Rina en Lian, door jullie
heldere blik heb ik geleerd dat het leven niet zo ingewikkeld hoeft te zijn als dat
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spelen of gewoon samen eten. Ik bedank ook mijn moeder, die er altijd voor ons
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Curriculum Vitae

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Academic Career

2015-2020 PhD at Photonics and Semiconductor Nanophysics group at Eindhoven University of Technology
Thesis: Active manipulation of the g-tensor in semiconductor nanostructures

2012-2015 Master Applied Physics at Eindhoven University of Technology
Thesis: Strain-induced g-factor tuning in individual InGaAs quantum dots

2009-2012 Bachelor Applied Physics at Eindhoven University of Technology
Thesis: Streak cavity for ultracold electron pulses

2003-2009 High school education (VWO) at Sondervick College, Veldhoven

Extracurricular

Since 2010 Co-organizer of Jeugd & Jongerenkamp, a yearly summer camp for mentally disabled young adults in the region of Eindhoven
List of publications

Journal papers


Conference talks

H.M.G.A. Tholen et al. - Strain-induced g-factor tuning in single InGaAs/GaAs quantum dots - International Conference on Quantum Dots, Jeju 2016

H.M.G.A. Tholen et al. - Active tuning of the g-tensor in InGaAs/GaAs quantum dots via strain - International Conference on the Physics of Semiconductors, Montpellier 2018

H.M.G.A. Tholen et al. - Active tuning of the g-tensor in InGaAs/GaAs quantum dots via strain - Physics@Veldhoven 2019

Conference posters

H.M.G.A. Tholen et al. - Strain-induced g-factor tuning in single InGaAs/GaAs quantum dots - International Winterschool on New Developments in Solid State Physics, Mauterndorf 2016

H.M.G.A. Tholen et al. - Strain-induced g-factor tuning in single InGaAs/GaAs quantum dots - Physics@Veldhoven 2018
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