OPTICAL PROPERTIES OF STRAINED, DISORDERED
InGaAs BASED SINGLE QUANTUM WELLS

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Abstract

In this thesis the results are presented of a theoretical investigation into the effects of strain and quantum well disordering (interdiffusion across the well-barrier interface) on the carrier confinement profiles and subband structure of strained InGaAs/GaAs undoped, single quantum wells and the resultant changes in their optical properties, including the absorption coefficient and the refractive index, which are of importance in photonic applications. An error function distribution is used for the constituent atoms composition after interdiffusion. The subband structure is calculated using spatially dependent effective masses and strain, within the parabolic band approximation and neglecting valence subband mixing. Excitonic effects and the continuum states below the barrier band edge are considered.

The results obtained show that disordering of InGaAs/GaAs quantum wells leads to graded strain and carrier confinement profiles. The ground state transition energy increases with interdiffusion so that the fundamental absorption edge shifts to shorter wavelengths, and can be tuned to wavelengths around 1 μm. For wavelengths > 1 μm the refractive index decreases as the extent of disordering increases, resulting in a positive refractive index step with respect to the as-grown region. This indicates the possibility of strong lateral confinement of photons in strained quantum wells.

Results are also presented showing how disordering modifies the exciton Stark shift that occurs when an external electric field is applied. They show that disordering can increase the Stark shift in InGaAs/GaAs quantum wells, leading to enhanced electroabsorption effects, and thus demonstrating the potential of improving device performance, such as a higher on/off ratio and a lower operational voltage, in electroabsorption modulators.

It is also shown that the disordering of In$_{0.55}$Ga$_{0.47}$As/InP quantum wells, combined with the strain that can arise, leads to confinement profiles which are quite distinct from those of both strained InGaAs/GaAs and lattice-matched AlGaAs/GaAs disordered quantum wells, and which could be of interest for photonic applications. An abrupt confinement profile is maintained after interdiffusion, with a potential build-up in the barrier near the interface, and miniwells at the bottom of the potential wells. Results show that the heavy hole well can support the ground state within the miniwells and that the potential build-up can result in quasi-bound states.
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Publications

Parts of this thesis have been published or accepted for publication:


### Acronyms

<table>
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<th>Acronym</th>
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<tr>
<td>CLT</td>
<td>Critical Layer Thickness</td>
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<tr>
<td>COP</td>
<td>Cross-Over Point</td>
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<tr>
<td>HH</td>
<td>Heavy Hole</td>
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<tr>
<td>IFVD</td>
<td>Impurity-Free Vacancy Diffusion</td>
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<td>IID</td>
<td>Impurity-Induced Disordering</td>
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<td>LH</td>
<td>Light Hole</td>
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<tr>
<td>MQW</td>
<td>Multiple Quantum Well</td>
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<tr>
<td>NSQW</td>
<td>Non-square Quantum Well</td>
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<tr>
<td>OEIC</td>
<td>Optoelectronic Integrated Circuit</td>
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<tr>
<td>PL</td>
<td>Photoluminescence</td>
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<tr>
<td>QCSE</td>
<td>Quantum-Confined Stark Effect</td>
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<tr>
<td>QW</td>
<td>Quantum Well</td>
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<tr>
<td>SEED</td>
<td>Self-Electro-Optic-Effect Device</td>
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<tr>
<td>SLS</td>
<td>Strained-Layer Superlattice</td>
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<tr>
<td>TE</td>
<td>Transverse Electric Mode</td>
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<tr>
<td>TM</td>
<td>Transverse Magnetic Mode</td>
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List of Symbols

a  hydrostatic deformation potential
a'' lattice spacing of strained layer in the interfacial plane
a_s exciton Bohr radius
a_o lattice constant of unstrained material
A_n,t coefficient for subband hole states expansion
c_{ij} elastic stiffness constants of epitaxial layers
c_o velocity of light
C\ell electron subband level
e electron charge
erf error function
E_b exciton binding energy
E_g bandgap edge
E_{cpwq} interband transition energy
E_{rc} confinement energy for carrier type r and level \ell
f lattice mismatch
F external applied electric field
G_i shear modulus of epitaxial layers
h_c critical layer thickness
H_i(z) Struve function of order 1
k_{||x} wave vector in direction of x-y plane
k_x wave vector in direction of x-axis
k_y wave vector in direction of y-axis
\ell 1, 2, 3, ...
L Brillouin zone end along <111> direction
L_d

L_z

L_{sq}

m_o

m^*_r

m^*_{\parallel r}

m^*_{\perp r}

M_{pq}

n

n_r

N_i(z)

p, q

Q_r

r
e (electron), c (conduction band), v (valence band), hh (heavy hole), lh (light hole)

R

s, s'

S(E)

U_{COP, r}

U_i(z)

V_i

x

x(z)

X

z

z_b

\frac{1}{2} L_b
$\alpha(\omega)$  optical absorption coefficient

$\alpha_{bo}(\omega)$  absorption coefficient for bound states

$\alpha_{1s}(\omega)$  absorption coefficient for 1S exciton

$\Gamma$  Brillouin zone centre <000>

$\Gamma_b$  half width half maximum broadening parameter

$\gamma_z$  Luttinger parameter

$\Delta_o$  spin-orbit splitting energy gap

$\varepsilon$  in-plane strain

$\varepsilon_1$  real part of dielectric constant

$\varepsilon_2$  imaginary part of dielectric constant

$\mu^*_{\text{cv}}$  electron-hole reduced effective mass

$\sigma$  Poisson's ratio

$\chi_{td}$  QW envelope wave function

$\chi_{1s}$  1S exciton envelope wave function

$\Psi_{td}$  QW wave function

$\Delta E_g$  bandgap offset

$\Delta E_r$  conduction or valence band discontinuity

$\beta$  variational parameter

$\delta$  delta function

$\lambda$  wavelength

$\rho$  2D position vector

$\omega$  angular frequency

$\mathcal{L}$  Lorentzian distribution

$\Theta^{TR, TM}$  polarisation factor

$h$  Planck's constant
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Chapter 1

INTRODUCTION

Optical communication, optical computing and signal processing, and optical interconnects are being extensively researched as they offer the potential of exploiting advantages associated with lightwave technology in general, namely, larger information capacities than electronic technology, the absence of electromagnetic interference, and parallel processing. Optical communication systems utilise optical fibres as the transmission line due to their enormous bandwidth and small propagation losses and require optical methods for signal multiplexing, demodulation and routing. Optical interconnects offer the potential for the rapid transfer of parallel data from one system to another without the problems of electromagnetic interference and signal dispersion commonly observed in high-bit-rate electrical interconnects. Modulatable light sources and optically addressable spatial light modulators are among the elements required in such an interconnect scheme. In optical computing systems there is also a need of optical bistable devices for optical binary logic gate applications.

Integrated optical devices have been developed which implement various functions with light such as modulation, switching, generation, and detection, in an optical guided wave structure formed on a substrate. Different material technologies have emerged as important for fabricating integrated optical devices. Lithium niobate has been widely investigated because it has a strong electro-optic effect, which is important for performing active functions such as modulation and switching,\textsuperscript{1,1} and because low loss waveguides can be fabricated. However, the use of lithium niobate precludes potential integration onto the same substrate with semiconductor lasers and high-speed electronic devices.
Compound III-V semiconductors such as AlGaAs (on GaAs substrates) and InGaAs(P) (on InP substrates) have been used to fabricate optical devices such as semiconductor lasers,\textsuperscript{1,2} detectors,\textsuperscript{1,3} low-loss optical waveguides,\textsuperscript{1,4} and high-speed electro-optic modulators,\textsuperscript{1,5,1,6} and have made the realisation of sophisticated device structures possible. For instance, wavelength tunable single mode lasers with a narrow optical linewidth, such as electronically tunable distributed feedback and distributed Bragg reflector lasers,\textsuperscript{1,7} have been designed for use in various applications, such as the local oscillator function\textsuperscript{1,8} in coherent optical fibre communications. High-speed electronic devices have also been fabricated in these III-V semiconductor compounds, indicating the possibility of integrating photonic and electronic devices onto the same substrate leading to optoelectronic integrated circuits (OEIC), such as integrated multichannel photoreceivers.\textsuperscript{1,9} OEICs offer the potential of improvement in performance and functionality as well as reduction of size and costs compared to hybrid circuits. This monolithic integration of electronic and photonic devices onto a single chip has, during the last several years, become the focus of considerable research effort as a direct response to the emerging fields of optical communication and optical computing.

Developments in semiconductor growth technology have enabled lattice-matched and strained quantum well (QW) structures to be fabricated which exhibit many unique material properties which cannot be realised in bulk semiconductors.\textsuperscript{1,10} These properties have resulted in improved optoelectronic devices as well as in completely new types of devices. For instance, the improvement in laser performance,\textsuperscript{1,10} such as lower threshold current density, operation at higher temperatures, modulation at higher frequencies and reduced spectral linewidths,\textsuperscript{1,11} is so dramatic that quantum well lasers are now available from a number of commercial sources. The novel self-electro-optic device (SEED) and related devices,\textsuperscript{1,12} which are proving of importance for optical signal processing and
computer applications, are possible because of the quantum-confined Stark effect, which is not observed in bulk semiconductors. Very large numbers of extremely small (~10 \( \mu \)m square) devices with low-power consumption can be fabricated permitting the realisation of highly parallel and complex optical architectures. For instance, a 64x32 array of symmetric SEED devices, each of which can be operated as a memory element or logic gate has been reported.\(^{1,13}\)

Despite considerable advances in QW integrated optical devices the goal of optoelectronic integration, which requires the fabrication of different device structures on adjacent areas of the substrate, is still in an early stage of development, since the various devices require different optical bandgap energies. The shifting of bandgap energies on a wafer to accommodate the different requirements usually involves complicated etch and regrowth techniques which are possible in principle but difficult in practice. The possibility of changing the constituent atoms composition in a QW by post-growth disordering has proved to be an additional attraction in using QW structures for photonic devices. The QW disordering process results in interdiffusion of the constituent atoms and leads to a change in the QW profile from an as-grown, square shape to a linearly graded profile, resulting in the possibility of continuous bandgap energy modification.\(^{1,14}\)

Two disordering techniques are being actively investigated for several III-V material systems: impurity-induced disordering\(^{1,15}\) and impurity-free vacancy diffusion.\(^{1,16}\) Both processes have been shown to disorder not only lattice-matched QWs such as AlGaAs/GaAs and In\(_{0.55}\)Ga\(_{0.45}\)As/InP, but also strained-layer structures such as InGaAs/GaAs. The disordering process can be localised to selected areas of the QW structures and can thus be an attractive tool of bandgap engineering with potential application for photonic and optoelectronic integration.
The greatest amount of work on QW properties and devices has been focused on AlGaAs/GaAs QW structures, helped by the relative ease of growth of this lattice-matched material system. However, AlGaAs/GaAs QW structures result in devices suitable for operations around 0.8 µm wavelength and other III-V material QW systems are being investigated for applications in the near infrared region, 1 µm to 1.55 µm wavelength range. The ternary layer InGaAs has attracted attention for photonic applications because it allows operation in this wavelength range and can be grown on both GaAs and InP substrates.

The lattice-mismatched InGaAs/GaAs material system is of interest because of the promising developments in strained InGaAs/(Al)GaAs quantum well lasers, which lase at a wavelength about 1 µm, and which offer the potential of having considerably lower threshold current than that of GaAs/AlGaAs QW lasers. In contrast to the AlGaAs/GaAs material system, the GaAs substrate in InGaAs/GaAs is transparent at the wavelength of the exciton absorption, which offers advantages in integrated laser applications, and in devices such as the spatial light modulator, where it is desirable to transmit the radiation in a direction perpendicular to the plane of the QW structure. InGaAs/GaAs exhibits a relatively low-barrier height in both conduction and valence bands potentially contributing to improved speed via reduced carrier extraction times, which is of interest in modulator applications. The InGaAs/GaAs material system has also been used to fabricate devices such as high electron mobility transistors and avalanche photodiodes, thus making InGaAs/GaAs attractive for monolithic optoelectronic integration.

Progress in epitaxial growth techniques using phosphorus has made it possible to obtain high-quality InGaAs(P)/InP QW structures. Lattice-matched In\textsubscript{0.55}Ga\textsubscript{0.45}As/InP QW structures are being investigated for a variety of optoelectronic
devices for operation in the 1.3 \( \mu \text{m} \) to 1.55 \( \mu \text{m} \) wavelength range, where future optical communication systems will likely operate as a result of the low loss and minimum dispersion characteristics exhibited by optical fibres in this wavelength range. The ability to grow InGaAs layers on InP substrates also provides a transparent substrate at these long wavelengths. It is also possible to fabricate devices such as junction field-effect transistors using In\(_{0.53}\)Ga\(_{0.47}\)As as the channel layer material, grown on an InP substrate,\(^1\)\(^2\)\(^5\) so that In\(_{0.53}\)Ga\(_{0.47}\)As/InP is also being investigated for applications in optoelectronic integration.\(^1\)\(^2\)\(^6\)

Both InGaAs/GaAs and In\(_{0.53}\)Ga\(_{0.47}\)As/InP QW structures are thus of interest for photonic applications, and selective disordering of these QW structures can prove a useful tool in modifying their optical properties. InGaAs/GaAs is a strained-layer material system and In\(_{0.53}\)Ga\(_{0.47}\)As/InP, which starts as an as-grown lattice-matched material system, can become strained as a result of disordering.\(^1\)\(^2\)\(^7\) In order to gain an insight into the potential use of disordering of strained QW structures for photonic applications it is useful to evaluate how the absorption coefficient and refractive index, which dominate the optical properties, of the strained QW structures vary with disordering.

The aim of this thesis is to model the effects of disordering on the optical properties of undoped, strained single QWs. In particular, the effects of strain and disordering on the subband structure of pseudomorphic InGaAs/GaAs and of In\(_{0.53}\)Ga\(_{0.47}\)As/InP single QWs are investigated, while the variation of the absorption coefficient and refractive index, as well as changes in the quantum-confined Stark shift and electroabsorption, caused by disordering are considered in detail for the InGaAs/GaAs material system. Strain and disordering modify the QW confinement profile and thus the subband structure, so that the interband transitions and the complex dielectric function of the QW are also varied, resulting in changes in the absorption
coefficient and refractive index at photon energies around and below the bandgap of the QW structure. The absorption coefficient is of interest in applications such as photodetectors and modulators, while changes in the refractive index are important for the confinement of photons and hence for waveguide applications, as well as for modulator and switching applications. The quantum-confined Stark shift is a fundamental characteristic that determines the performance of optical modulators.

The thesis is arranged as follows: in chapter 2 a brief review is presented on strained-layer structures, QW confinement profiles and disordering of QWs. For photonic applications a strained-layer structure must be coherently strained and this entails a critical (maximum) thickness for the layers. The strain induced in a coherently strained QW structure is influenced by the composition of the buffer layer between the structure and the substrate, as well as by the thickness and composition of the structure itself. The effects of this strain on the band structure at the Brillouin zone centre are briefly discussed for square QWs, followed by the properties and potential applications of square and some non-square QW confinement profiles. A brief review of impurity-induced disordering and of disordering by impurity-free vacancy diffusion concludes the chapter. In chapter 3 the effects of strain and disorder on the confinement profile and subband structure of single InGaAs/GaAs QWs are investigated. An error function compositional distribution is assumed after disordering. Details of the theoretical considerations used in the model are presented and the numerical results obtained are presented and discussed.

Chapter 4 deals with the variation of the absorption coefficient with disordering of InGaAs/GaAs single QWs. Results are presented firstly for the polarisation dependent absorption coefficient spectrum for interband transitions, taking into account valence subband mixing, and secondly for the absorption coefficient spectra for light propagating
normal to and along the plane of the QW, using the parabolic band approximation and taking into consideration the 1S-like exciton and all bound states. It is shown that the exciton peaks in TE polarisation remain constant with disordering, and that the absorption edge, which shifts to shorter wavelengths with disordering, can be tailored to desired wavelengths around 1.0 \( \mu \text{m} \). The variation with disordering of the polarisation dependent refractive index of disordered InGaAs/GaAs single QWs, calculated for the wavelength range 0.87 \( \mu \text{m} \) to 2 \( \mu \text{m} \), using the complex dielectric function, is presented in chapter 5. The results show that a positive lateral refractive index step is obtained when the lateral confining regions are more extensively disordered, indicating that photon confinement is possible in strained QW structures. The effects of disordering on the quantum-confined Stark shift and electroabsorption properties of InGaAs/GaAs single QWs are investigated in chapter 6. The results indicate that, compared to an as-grown QW, an increased Stark shift can be achieved as a result of disordering, leading to enhanced electroabsorption effects, which could improve the performance of optical modulators. In chapter 7, the model developed for the subband edge structure for disordered, strained InGaAs/GaAs QWs is applied to disordered In\(_{2.5}\)Ga\(_{0.47}\)As/InP single QWs. It is shown that an interesting confinement profile results, when considering cation interdiffusion only, which differs from that of disordered AlGaAs/GaAs and InGaAs/GaAs QWs. An abrupt confinement profile is maintained even after significant interdiffusion, while a potential build-up occurs in the barrier near the interface and miniwells arise inside the potential wells. The subband edge structure shows that the potential build-up can result in quasi-bound states, while the heavy hole well can support the ground state within the miniwells, which may be of use in electronic and photonic applications. Chapter 8 summarises the conclusions of the thesis and gives suggestions for further work.
References


Chapter 2

STRAINED QUANTUM WELL STRUCTURES

The development of new material growth technologies such as molecular beam epitaxy,\textsuperscript{2,1} and metalorganic vapour phase epitaxy,\textsuperscript{2,2} has made possible the growth of semiconductor microstructures whose dimensions are comparable to atomic dimensions and whose interfaces are atomically smooth. Quantum well structures consist of alternating ultrathin layers, for instance 10 nm thick, of two different semiconductors, such as AlGaAs/GaAs,\textsuperscript{2,3} and In\textsubscript{0.53}Ga\textsubscript{0.47}As/InP.\textsuperscript{2,4} Since the lattice parameters of the adjacent semiconductors in these material systems are very similar the QW structures are lattice-matched. It is also possible to grow high-quality strained-layer structures, where adjacent layers in the heterostructure do not have matching lattice constants. This freedom from the need for precise lattice matching widens the choice of compatible materials, and increases the ability to control the optical and transport properties of QW structures. As a result various strained-layer material systems, such as InGaAs/GaAs,\textsuperscript{2,5} strained In\textsubscript{2}Ga\textsubscript{1-x}As/InP,\textsuperscript{2,6} and GaAsP/GaP,\textsuperscript{2,7} are being widely investigated for photonic and electronic applications.

2.1. Strained-Layer Structures

When a film is grown epitaxially on a substrate with a different lattice constant, the lattice mismatch can be accommodated by different mechanisms, see Fig. 2.1. The major mechanisms\textsuperscript{2,8} include: dislocation generation at the interface, coherent strain, metastable epitaxy (a combination of strain and misfit dislocations), bending of the
epitaxial layer, and tilt of the lattices with respect to each other. In optoelectronic devices, dislocations in the active region are undesirable. It is, therefore, important to realise conditions in which no misfit dislocations are present, so that the structure is coherently strained. The individual layers in such a strained-layer structure match up the lattice constants in the plane parallel to the interface by compression or expansion in this plane. A tetragonal deformation in the layers also takes place so that the layers are compressed or expanded in the direction perpendicular to the interfacial plane. Thus the resultant strains in a coherently strained structure consist of a biaxial hydrostatic strain parallel to the interface and a uniaxial shear component parallel to the direction of epitaxial growth.

2.1.1. Pseudomorphic Quantum Well Structures

The strain induced in a strained-layer structure is influenced by the composition of the buffer layer between the strained-layer structure and the substrate. For instance, an In$_x$Ga$_{1-x}$As/GaAs strained-layer superlattice (SLS) can be grown on a compositionally-graded In$_x$Ga$_{1-x}$As buffer layer lattice matched to the unsupported in-plane lattice constant of the superlattice. In this case the alternate layers match up the lattice constants in the plane parallel to the interface so that the GaAs layer is under tension and the In$_x$Ga$_{1-x}$As layer is under compression, Fig. 2.2. For such a superlattice its in-plane lattice spacing, $a''$, is between the unstrained lattice constant of GaAs and In$_x$Ga$_{1-x}$As, and is given by

$$a'' = a_0 \left[1 + \frac{f}{1 + G_f h_2/G_f h_2}\right]$$  

(1)
Fig. 2.1. Schematic illustration indicating major ways by which lattice mismatch is accommodated in heteroepitaxial growth. All of the mechanisms have been observed experimentally.\(^{2,8}\)
Fig. 2.2. Schematic diagram of $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLS grown on an $\text{In}_y\text{Ga}_{1-y}\text{As}/\text{GaAs}$ buffer layer.
where $a_1$ is the unstrained lattice constant of layer 1, $h_1$ and $h_2$ are the thickness of the individual superlattice layers, $f$ is the lattice mismatch of the unstrained layer materials, and $G_1$ and $G_2$ are the shear moduli of the two layers, given by \(^2\)\(^{11}\)

$$G_i = 2[c_{i1}^1 + c_{i1}^2 - 2(c_{i2}^2/c_{11}^1)] \quad i = 1, 2$$

(2)

where $c_{11}^1, c_{12}^1 (c_{11}^2, c_{12}^2)$ are the elastic stiffness constants of the two layers.

The compressive in-plane strain $\varepsilon$ in the InGaAs layer is given by \(^2\)\(^{14}\)

$$\varepsilon = (a'' - a_{\gamma}(x))/a_{\gamma}(x)$$

(3)

where $a_{\gamma}(x)$ is the lattice constant of bulk In\(_x\)Ga\(_{1-x}\)As, obtained by linear interpolation between the binary data.\(^2\)\(^{15}\) It can be seen that the strain depends on the in-plane lattice spacing of the SLS, which in turn depends on the indium content $x$, and the ratio of the layer thicknesses.

Alternatively, InGaAs/GaAs superlattices can be grown on a GaAs buffer layer, such that the resultant SLS in-plane lattice spacing matches the GaAs lattice constant.\(^2\)\(^{12}\)

In this pseudomorphic structure the ternary layer is under (compressive) strain, whereas the binary layer is unstrained.\(^2\)\(^{12}\) The compressive in-plane strain $\varepsilon$ in the InGaAs layer is\(^2\)\(^{16}\)

$$\varepsilon = (a_{\gamma\text{GaAs}} - a_{\gamma\text{InGaAs}})/a_{\gamma\text{InGaAs}}$$

(4)

where $a_{\gamma\text{GaAs}}$ is the lattice constant of bulk GaAs, and $a_{\gamma\text{InGaAs}}$ is the lattice constant of bulk In\(_x\)Ga\(_{1-x}\)As. Thus for pseudomorphic structures the strain in the InGaAs layer is a direct function of the indium content and is independent of the thickness of the layer.\(^2\)\(^{17}\)

It can be seen from equation (3) and (4) that InGaAs layers in pseudomorphic
InGaAs/GaAs structures have a higher compressive strain than InGaAs layers in a structure grown on an In$_y$Ga$_{1-y}$As buffer layer. Pseudomorphic structures are advantageous in photonic applications since dislocations which arise at the graded buffer-substrate interface are avoided.

### 2.1.2. Critical Layer Thickness

For a small enough lattice mismatch in a heterostructure (less than about 3%),$^{2,18}$ there is a critical layer thickness (CLT),$^{2,14}$ below which dislocations are not generated because it is energetically more favourable to accommodate the strain energy by stretching the epitaxial layer than to create dislocations. There have been a number of calculations of the CLT,$^{2,14,2,19,2,20}$ and there is some controversy regarding the determination of CLTs. The force-balance model developed by Matthews and Blakeslee$^{2,14}$ and the energy-balance model developed by People and Bean$^{2,19}$ have both gained experimental support despite predicting values of CLTs which differ by as much as an order of magnitude. The force-balance model supposes that the strain relaxation in the epitaxial layer is entirely determined by the dynamics of threading dislocations which can move under the resultant forces acting on them. The CLT is considered to be the layer thickness in which the force due to the misfit strain on an existing grown-in threading dislocation equals the tension in the dislocation line. For a structure such as In$_x$Ga$_{1-x}$As/GaAs the CLT can be written as$^{2,18}$

$$h_c = \frac{a}{\sqrt{2}} \frac{1}{4\pi f} \frac{1 - \sigma/4}{1 + \sigma} \left[ 1 + \ln \left( \frac{h_c \sqrt{2}}{a} \right) \right]$$

where $f$ is the mismatch, $a$ is the lattice constant of the In$_x$Ga$_{1-x}$As, and $\sigma$ is Poisson’s ratio. Misfit accommodation by half-loop nucleation gives results for the CLT which are
almost identical to the threading dislocation results. The above expression for \( h_e \) relates to a single epilayer structure. The CLT for a multilayer structure differs by a factor of 4. The energy-balance model, which predicts values of \( h_e \) larger than those found using eq. (5), assumes that the growing film is initially free of threading dislocations, and that the interfacial misfit dislocations will be generated when the areal strain density exceeds the energy density associated with the dislocation-generating mechanism which is of minimum energy. The model neglects the movement of threading dislocations so that it is valid only when the density of dislocations in the substrate is very low. The CLT calculated with this model is given by

\[
h_e = \frac{a}{\sqrt{2}} \frac{1}{32 \pi f^2} \frac{a}{(1 + \sigma)} \left[ \ln \left( \frac{h_e \sqrt{2}}{a} \right) \right]
\]  

It can be seen from equation (5) and (6) that the CLT is a function of the mismatch \( f \), and thus it is dependent on the composition of the layers in the structure. For pseudomorphic \( \text{In}_x\text{Ga}_{1-x}\text{As/GaAs} \) QW structures, the CLT of the \( \text{In}_x\text{Ga}_{1-x}\text{As} \) layer decreases as the In composition \( x \) increases. \( \text{In}_x\text{Ga}_{1-x}\text{As/InP} \) QW structures are lattice-matched for an In composition \( x = 0.53 \). For \( x < 0.53 \), the \( \text{In}_x\text{Ga}_{1-x}\text{As} \) layer is under tension, with the strain increasing as \( x \) decreases. For \( x > 0.53 \), the \( \text{In}_x\text{Ga}_{1-x}\text{As} \) layer is under compressive stress, with the modulus of the strain increasing as \( x \) increases. Thus starting from the lattice-matched \( x = 0.53 \), the CLT of \( \text{In}_x\text{Ga}_{1-x}\text{As} \) layers in pseudomorphic \( \text{In}_x\text{Ga}_{1-x}\text{As/InP} \) QW structures decreases both as \( x \to 0 \), and as \( x \to 1.0 \). The difference in the predictions for the CLTs between the force-balance model and the energy-energy model are shown in Fig. 2.3, for \( \text{In}_x\text{Ga}_{1-x}\text{As/GaAs} \) heterostructures.
Fig. 2.3. Calculated curves of critical layer thickness as a function of indium composition for InGaAs on GaAs.
Low temperature photoluminescence (PL) spectra have been widely used to study the quality of strained-layer structures. Sharp PL peaks attest to high quality of the structures, and the full wave half maximum (FWHM) of the spectra is used as a figure of merit reflecting the heterointerface quality. CLTs of QWs have been determined using PL spectra since, when the QW width approaches the critical thickness value, the PL peak shifts to lower energy, broadens, and decreases in intensity, indicating the appearance of additional dislocations. These dislocations in the structure act as non-radiative recombination centres, thereby reducing the PL intensity and modifying the PL response. CLTs have been measured using other experimental techniques such as x-ray diffraction and transmission electron microscopy (TEM) micrographs. Differences in the experimental resolution of the various experimental techniques used for the measurement of CLTs have been cited as contributing to the wide discrepancy in the measured values of critical thicknesses. Comparison of theory and experiment is further complicated by the possibility of a metastable region in which high-quality layers with thickness greater than the CLT may be grown. The usefulness of these layers will depend on the particular device application. For example, absorption-based devices would perform reasonably well in this region, while the performance of strained layer QW lasers would be very sensitive to the quality of the strained layer. In the InGaAs/GaAs material system, Fritz et al. and Andersson et al. using PL measurements, have reported measured CLTs which agree well with the theoretical expression proposed by Matthews and Blakeslee, while Orders and Usher, using x-ray diffraction, reported much larger CLTs, in good agreement with the model of People and Bean. The maximum thickness for coherently strained layers is reported to depend strongly on the growth temperature, with increasing with decreasing substrate temperature. The CLT in strained InGaAs/InP QWs has been investigated by
Temkin et al.\textsuperscript{2,6} and the data reported shows that the CLTs in this material system are again determined by the Matthews and Blakeslee model.

2.2. Effects of Strain on the Band Structure.

The energy band structure of a semiconductor plays a fundamental role in determining its optical properties. Energy versus wave vector diagrams ($E$-$k$ dispersion relationships) are used to characterise the conduction and valence bands in crystals. In III-V semiconductors three degenerate $|p\rangle$-like valence bands attain an energy maximum at the $\Gamma$ point, the Brillouin zone centre ($k = 0$), while the $|s\rangle$-like lowest conduction band has a minimum at the $\Gamma$ point. The energy bands are affected by the interaction between the spin angular momentum and the orbital angular momentum of the electron. The result of this spin-orbit coupling is to remove orbital degeneracies, Fig. 2.4. The valence band states split by an amount $\Delta_{so}$, the spin-orbit splitting gap, the doubly degenerate $J = 3/2$ state moving up by $\Delta_{so}/3$ and the single ($J = 1/2, m_J = \pm 1/2$) state moving down by $2\Delta_{so}/3$,\textsuperscript{2,28} where $J$ is the total angular momentum quantum number and $m_J$ is the magnetic quantum number. The two degenerate bands have different curvatures at the $\Gamma$ point, so they are differentiated by the terms heavy-hole ($J = 3/2, m_J = \pm 3/2$) and light-hole ($J = 3/2, m_J = \pm 1/2$) bands.

Within the critical thickness regime, growth of In$_x$Ga$_{1-x}$As layers on (001) oriented GaAs substrates,\textsuperscript{2,29} or on (001) oriented InP substrates,\textsuperscript{2,30} results in coherently strained structures, (except for In$_{0.53}$Ga$_{0.47}$As/InP which is lattice-matched) so that as indicated above both biaxial hydrostatic and uniaxial shear strain are present. The biaxial strain does not alter the symmetry of the original crystal and its effect is to alter the band structure by shifting band-edge energies. The uniaxial strain lowers the symmetry of the crystal from that of unstrained bulk materials, splitting the degeneracy...
Fig. 2.4. Band structure at the Γ point for a direct-gap semiconductor showing valence band with spin-orbit splitting.
of the $J = 3/2$ state, and also produces a stress-induced coupling between the $m_f = \pm1/2$ bands (light hole and spin-orbit split-off bands).\textsuperscript{2,31} A compressive hydrostatic strain causes the in-plane atoms to get closer so that the conduction and valence band extrema move away from one another and the bandgap increases. The uniaxial strain lifts the degeneracy of the heavy hole (HH) and light hole (LH) subbands at the $\Gamma$ point, so that the HH band moves towards the conduction band edge and the LH band moves away from the conduction band edge,\textsuperscript{2,32} Fig. 2.5. In the case of tensile strain, the in-plane atoms move away and the opposite situation arises. The hydrostatic strain causes a decrease in the bandgap while the uniaxial strain moves the HH away from the conduction band edge and the LH band towards the conduction band edge, Fig. 2.5.

A sketch of the variation of the change in HH and LH bandgap energy with indium content, for strained In$_x$Ga$_{1-x}$As is shown in Fig. 2.6.\textsuperscript{2,33} As the indium content increases, the in-plane (compressive) strain and the bandgap energy for the HH and the LH increases. The lifting of the HH and LH degeneracy can be observed, and as the indium content increases the difference between the HH and LH bandgap energy also increases, as the effect of the uniaxial strain becomes more pronounced. This increase in separation between the HH and LH bandgap energies strongly influences the optical response of strained QW structures.

Strain also induces anisotropy in the hole effective masses.\textsuperscript{2,34} The splitting between the HH and LH states alters the band-to-band mixing and, consequently, changes the parallel effective masses. For compressively strained layers $m_f = 3/2$ holes become heavy in the growth direction and comparatively light in the layer plane, and the $m_f = 1/2$ holes become light in the growth direction and comparatively heavy in the layer plane.\textsuperscript{2,35} This is indicated schematically by the band curvatures in Fig. 2.5. (In this
Fig. 2.5. A schematic illustration of the effects of strain on the band structure at the $\Gamma$ point. (a) the band structure of the unstrained material, showing the HH ($V_1$) and LH ($V_2$) bands degenerate at $\Gamma$ point. (b) biaxial compressive strain increases the bandgap, with the HH band being the highest lying valence band. The comparatively light hole nature of this band in the plane of the well ($k_{\|}$) is indicated. (c) the effects of biaxial tension are similarly illustrated.
Fig. 2.6. Calculated increase in heavy-hole and light-hole bandgap in compressively strained InGaAs.
thesis references to HH and LH assume the direction of growth and thus refer to \( m_r = \frac{3}{2} \) and \( m_r = \frac{1}{2} \) holes, respectively.

### 2.3. Square Quantum Well Confinement Profiles

#### 2.3.1. Lattice-Matched Quantum Wells.

When semiconductor A is grown epitaxially on semiconductor B with a very sharp compositional transition from A to B at the interface (within a few lattice constants) an abrupt heterojunction is formed. Fig. 2.7(a) shows a schematic diagram of the band structure at \( \Gamma \) of a lattice-matched QW with a narrow band gap material, A, surrounded by a wider band gap material, B. This could be for example \( \text{In}_{0.53}\text{Ga}_{0.47}\text{As} \) (A) and InP (B). In the as-grown structure abrupt discontinuities at the heterojunction at both the conduction-band edge and valence-band edge at \( \Gamma \) give rise to square potential wells in both the conduction band and the valence band. The narrow band gap material acts as the well while the wider band gap material acts as the barrier. The width of the square potential wells is equal to the thickness of the narrow band gap material, while the depth of the potential wells depends on the band offsets for the QW material system.

In the growth direction, electrons are confined to the conduction potential well and holes are confined to the valence potential well. For well widths less than the de Broglie wavelength, quantization occurs and results in a series of discrete energy levels inside the well.\(^{236}\) The position of these energy levels depends on the depth and width of the potential well, that is on the carrier confinement profile. The wavefunction and energies of the confined (subband) states are indicated in Fig. 2.7(a).
Fig. 2.7. (a) The energy and wavefunction, $\Psi$, of some of the subband states for a lattice-matched QW, are indicated. For clarity, the heavy hole and light hole wells are shown separately. $\ell$ labels the confined levels in each well. (b) The construction of the total energy of an electron in the conduction band of a QW structure; $z$ is the growth direction. The two dimensional density of states $\rho(E)$ is also shown (the broken line illustrates $\rho(E)$ for a bulk semiconductor).
In the perpendicular direction, in the plane of the well, there is no such effect. The \( E-k \) dispersion curves remain that of the bulk material so that, for example, the total energy of an electron in the first subband state may be written as

\[
E_L + \frac{\hbar^2 k_{||}^2}{2m_e^*}
\]  

(7)

where \( k_{||} \) is the wave vector in the plane of the QW, \( m_e^* \) is the effective mass of the electron, and \( E_L \) is the confinement energy found by solving the one-dimensional Schrödinger equation, written with respect to the bulk conduction edge. This is shown in Fig. 2.7. This combination of discrete energy levels and free electron-like dispersion curves leads to a step density of states, also illustrated in Fig. 2.7(b), each step originating from the onset of a subband. The detailed form of the staircase curve can be tailored by controlling the material composition, and the QW structure parameters such as well width and/or barrier thickness. The parabolic three dimensional density of states is shown by the dashed line. An important consequence of this is that the density of states at the bottom of the conduction band in a QW is finite whereas in a bulk material it is zero. This has important, useful consequences for some devices such as QW lasers.

### 2.3.2. Strained Quantum Wells

Consider now a pseudomorphic InGaAs/GaAs QW structure, where the InGaAs layer is compressively strained. As already noted, the hydrostatic compressive strain increases the bandgap of the InGaAs layer at \( I \), and the uniaxial strain shifts the HH band edge towards the conduction band edge and moves the LH band edge away from the conduction band edge. The HH and LH confinement profiles no longer coincide and the depth of the HH confinement profile is larger than the LH confinement profile,
Fig. 2.8. In addition strain can also cause a different spatial situation to arise for the heavy and light holes. In the case of the HH, the conduction-band QW and the heavy hole QW will both lie in the InGaAs layer, and the electron and HH are both confined to this layer. Such a system is said to be of type I. In the case of the LH, the large increase in energy gap caused by the strain may result in the GaAs layer becoming the well and the InGaAs layer becoming the barrier for the LH. Such a system, where electrons and holes are spatially separated, is said to be of type II, Fig. 2.8. Different experimental groups have attributed the LH valence band to the InGaAs layer or to the GaAs layer.

The spatial situation of holes is strongly dependent on the value of band offsets. This is still, however, a vexed question for most III-V heterojunctions. The bandgap offset $\Delta E_g$ in a semiconductor heterojunction defines the energy difference between the respective bandgaps (conduction-band minimum to valence-band maximum at $\Gamma$) of the two layers forming the heterostructure, and is the sum of the conduction-band discontinuity $\Delta E_c$ and the valence-band discontinuity $\Delta E_v$ (Fig. 2.8(a)). The conduction band offset $Q_c$ is defined as $Q_c = \Delta E_c/\Delta E_g$ while the valence band offset $Q_v$ is defined as $Q_v = \Delta E_v/\Delta E_g$. The conduction-band discontinuity in the InGaAs/GaAs heterojunction has been determined experimentally using various techniques, including low-temperature PL spectra, room temperature photoreflectance spectra, and optical transmission measurements. A wide range of results have been reported for the conduction band offset $Q_c$ giving both a concentration dependent offset, as well as an offset that is independent of the indium concentration, but with $Q_c$ values varying from 0.30 to 0.83.
Fig. 2.8. Possible conduction- (C.B.) and valence-band (V.B.) confinement profiles of a strained InGaAs/GaAs quantum well structure. The valence band is split into heavy- (hh) and light-hole (lh) bands.
In$_{0.55}$Ga$_{0.45}$As/InP is another material system where a large discrepancy exists in reported band offset values determined through different experimental techniques.\textsuperscript{2,46} Early determinations based on optical spectroscopy indicated a $Q_c$ of about 0.65\textsuperscript{2,47} while measurements using capacitance-voltage data indicated a $Q_c$ of about 0.40.\textsuperscript{2,48} More recent reports on $Q_c$ measurements indicated a value of about 0.33,\textsuperscript{2,49,2,50} while a value of 0.40 has been used to provide an adequate fit to exciton peak energies in this material system as a function of QW width.\textsuperscript{2,51}

Thus, it can be seen that the question of the band alignment at the InGaAs/GaAs and In$_{0.55}$Ga$_{0.45}$As/InP heterojunctions has not yet been resolved. Nevertheless, the band offsets constitute an important parameter affecting the optical properties of a QW structure. The lowest, direct bandgap in an InGaAs/GaAs QW structure is the (interband) transition energy between the ground state in the conduction and HH valence band. The principal transition energy is therefore dependent on the strain and quantization effects. By altering the QW width or the ternary alloy composition the conduction and valence band confinement profiles are altered. As a result the position of the confined subbands is changed, and with it the principal interband transition energy, as well as higher order interband, transition energies, of the QW structure. Thus QW structures offer a wider range of principal transition energies than that possible by the use of bulk materials. Strained QW structures offer an extra degree of flexibility in tailoring the interband transition energies, and hence the optical properties, of a structure by making use of both strain and quantization effects.

2.4. Non-square Quantum Well Confinement Profiles

Square QW structures have been shown to be more promising than bulk materials for several device applications because they show well-resolved excitons at room
temperature, they have strong nonlinear optical effects associated with absorption saturation, they exhibit the quantum-confined Stark effect (QCSE), and show enhanced excitonic electrorefraction among other properties. These QW effects have been demonstrated in several III-V material systems, including AlGaAs/GaAs, InGaAs/InP, and InGaAs/GaAs, and have been exploited in various device applications such as photodetectors, waveguides, lasers, transverse and waveguide type modulators, and the self-electro-optic device (SEED) which relies on simultaneous optical modulation and optical detection. Square QWs, however, offer only limited possibilities in tuning optical properties. In a lattice-matched square QW the well and/or barrier thickness are normally the only relevant parameters in tailoring its properties. In a strained QW, strain provides an extra degree of freedom. More flexibility in customising the subband-structure dependent optical properties is possible in non-square quantum well (NSQW) structures.

Several different NSQW confinement profiles have been investigated, including step profiles, linearly and non-linearly graded profiles, or a combination of these types. A selective rather than a comprehensive overview follows intended to highlight distinctive effects of some NSQW structures which have been predicted theoretically or demonstrated experimentally.

2.4.1. Linear Profiles

An early study of the effect of compositional grading on the confined subband states was carried out using an AlAs-GaAs-AlAs QW heterostructure with linear compositional grading having a trapezoidal well shape (see Fig. 2.9). Calculations using the tight-binding method showed that the magnitudes of the confined energy levels increase with increasing graded region widths. The shifts reported due to the linearly
Fig. 2.9. A schematic diagram of the conduction and valence band edges of an Al-Ga-As quantum well heterostructure with linear compositional grading. $E_{lh}$, $E_{hh}$, $E_{ce1}$, $E_{ce2}$ are the light-hole, heavy-hole, ground state conduction, and second conduction band quantum well energies.\textsuperscript{276}
graded heterojunction indicated significant increases in the energy of the ground state (around 30%) and of the first excited state (around 19%) in the conduction band when compared to an equivalent square well. The compositional grading resulted in a measurable effect on both interband and intersubband transition energies. For example, the heavy-hole to conduction band transition energy increased by 29 meV; the intersubband transition energy from the ground state to the first excited state in the conduction band increased by 42 meV. It was thus shown that compositional grading can have a significant effect on the energy of the subband states, both in the conduction and in the valence bands.

A fundamental difference between the graded and abrupt interface is that the graded barrier height can be lowered or raised by the application of an electric field, whereas the abrupt barrier is less changed since a finite electric field produces no potential change in the vanishingly small distance of the abrupt interface, as shown in Fig. 2.10. Theoretical studies for asymmetric triangular QWs show that the shift in the fundamental absorption edge is approximately linear with the applied field strength and that the absorption spectrum tends to shift rigidly without losing its overall shape, in contrast to the square QW case, where the shift in fundamental absorption edge is nonlinear with field strength, and where the shape of the absorption spectrum varies in a complicated manner due to the growth and decay of the strength of the forbidden exciton lines. Symmetric and asymmetric triangular AlGaAs/GaAs QWs have been investigated experimentally and showed significant electroabsorption changes due to the quenching of the ground state induced by a sufficiently large electric field. The elimination of the graded barriers needed for quantum confinement by the field is responsible for the quenching of the excitonic absorption. Asymmetric triangular wells in the strained InGaAs/GaAs material system have also been recently investigated.
Fig. 2.10. Energy band diagrams of undoped symmetric and asymmetric triangular quantum well structures showing barrier lowering by different applied electric fields. $\Delta E_c$ and $\Delta E_v$ are the well depths in the conduction and valence bands, respectively.\textsuperscript{277}
The optical efficiency of such a structure, as reflected in normalised photoluminescence intensity measurements at 2K, was reported to be more than five times that of an equivalent square QW grown under the same conditions.

In order to achieve high device performances, such as high on/off ratio and low operating voltage, in high-speed optical modulators, it is desirable that a large Stark shift of the exciton is exhibited with applied electric field and that the decrease of exciton oscillator strength with applied field be small. A QW structure with a compositionally graded well bottom (Fig. 2.11) has been proposed for this purpose. Theoretical studies of this QW structure predict that the change in energy for the ground state exciton in the graded gap QW is always greater than that in a square QW in the presence of a positive electric field, where the electric field direction is considered positive when the valence-band edge becomes more inclined. On the other hand, the ground state exciton oscillator strength in the graded gap QW is almost the same as in the square QW, see Fig. 2.11. The results also show that a blue shift of the ground state exciton transition results when a negative electric field is applied. This effect has been developed to show theoretically that optical bistability is possible in a SEED with a single asymmetric QW having a graded gap profile.

2.4.2. Nonlinear Profiles

The first successful fabrication of layered structures of GaAs and Al$_x$Ga$_{1-x}$As to simulate a parabolic band profile between the confining Al$_x$Ga$_{1-x}$As layers were obtained by varying the layer thicknesses quadratically with the distance from the centre of the sample. Results showed that the subband states were almost uniformly spaced in energy reflecting a uniformly spaced density-of-states function for the electrons and holes. Interband and intersubband optical transitions in a parabolic QW with an applied
Fig. 2.11. (a) Schematic band diagram of the graded gap quantum well structure. (b) Electric field dependence of the transition energies and oscillator strengths of the ground state excitons (associated with the ground state HH1-E1 and LH1-E1 interband transitions) in the graded gap (solid lines) and square (dashed lines) quantum wells.²⁸²
field have been studied. The absorption spectrum for the intersubband transitions is insensitive to the applied field since all the subbands in the parabolic QW are shifted by an equal amount and the wavefunctions are all displaced by an equal distance, see Fig. 2.12. This is in contrast to the case of a square QW for which the Stark shift is a function of the eigen energy state. The absorption coefficient and refractive index change for the TE polarisation due to intersubband transitions in a parabolic QW are shown in Fig. 2.12, while the absorption coefficient and refractive index change as a function of applied field due to interband transitions are shown in Fig. 2.13, indicating a strong electro-optic effect.

The possibility of using parabolic QW structures for infrared detector application, based on absorption due to intersubband transitions, has been investigated. Superlattices made of parabolic QWs have the interesting feature that the ground state sees a wider barrier than the excited states due to the shape of the confining potential (Fig. 2.14) so that the ground states are nearly isolated from each other. This offers the possibility of lower leakage current due to tunnelling compared to square well superlattices with the same barrier thicknesses.

The NSQW confinement profiles discussed above result from compositional grading during epitaxial growth. While complex NSQW structures can be obtained by careful control of the material growth process in lattice-matched QWs, it is a much more difficult proposition in the case of strained QW structures. An alternative approach is to modify the compositional profile of square QWs after the epitaxial growth process. Selective disordering of QW structures is the post-growth technique that has attracted major attention and which is being widely investigated experimentally for the modification of QW confinement profiles and optical properties of both lattice-matched and strained QW structures.
Fig. 2.12. (a) Normalised energy levels $E_n$ as functions of normalised electric field $\tilde{F}$ for parabolic (solid lines) and square (dashed lines) quantum well. The width of the square well and the curvature of the parabolic well are chosen such that their ground state energies at $F = 0$ are equal for comparison.$^{2,86}$ (b) The absorption coefficient and refractive index change $\Delta n$ due to intersubband transitions in a parabolic quantum well. A curvature parameter $K_e = 1.64 \times 10^{11}$ eV/cm$^2$ and a linewidth $\Gamma_b = 10$ meV are used.$^{2,86}$
Fig. 2.13. The absorption coefficient and the refractive index change $\Delta n$ due to interband transitions as a function of electric field for a parabolic quantum well.\textsuperscript{286}
Fig. 2.14. (a) Schematic diagram of a parabolic quantum well showing the intersubband transition; (b) Parabolic well superlattice showing the isolated ground state and miniband at the first excited state.$^{288}$
2.5. Disordering of Quantum Wells

Techniques such as etch and regrowth have been successfully used\textsuperscript{2.89} for bandgap modification, but only two values of bandgap energies result from such a process and the potential for bandgap modification is therefore somewhat limited. Disordering of QW structures, which involves the interdiffusion of constituent atoms across the well-barrier interfaces, is of particular interest since it offers the possibility of continuous modification of the material bandgap.\textsuperscript{2.90} Moreover the disordering process can be localised to selected regions of a QW structure so that the optical properties of only the selected areas are modified by the disordering process. Disordering has been successfully used to obtain very low threshold currents in strained InGaAs/GaAs QW lasers.\textsuperscript{2.91} A two-wavelength demultiplexing $p$-$i$-$n$ photodetector using disordered multiple QW structures has been demonstrated.\textsuperscript{2.92} The changes in refractive index that result from disordering of QW structures by different impurity species are under continuous investigation\textsuperscript{2.93,2.94} and have been used to fabricate devices such as optical channel waveguides\textsuperscript{2.95,2.96} which can selectively confine TE and TM modes, and QW buried heterostructure waveguides.\textsuperscript{2.97,2.98} The possibility of modifying the optical properties of selected areas also enables optical devices such as lasers, waveguides, modulators and optical switches to be integrated on the same chip, opening up the potential for photonic and optoelectronic integration.\textsuperscript{2.99} For instance, monolithic integration of a transparent dielectric waveguide into an active laser cavity by impurity-induced disordering has been demonstrated.\textsuperscript{2.100} Selective disordering of a multiple QW structure enables the integration of a laser and phase modulator, which requires modification of the modulator section to make it efficient at the lasing wavelength.\textsuperscript{2.101}

The two major processes that have been employed to disorder QW structures are impurity-induced disordering,\textsuperscript{2.102} and impurity-free vacancy diffusion.\textsuperscript{2.103,2.104} Thermal
annealing of III–V semiconductor heterostructures can result in the interdiffusion of constituent atoms across the well-barrier interface if the annealing is carried out at a suitably high temperature and for a sufficiently long time.\textsuperscript{2,0,2,05} In impurity-induced disordering, surface diffusion or ion-implantation of an impurity species is used to enhance the interdiffusion process. Zn diffusion has been widely investigated in both lattice-matched QW structures grown on GaAs and InP substrates,\textsuperscript{2,0,6-2,0,9} and strained-layer QW structures,\textsuperscript{2,1,0} and has been shown to greatly enhance the interdiffusion of group III atoms across the interface, thereby disordering the QW structure. Disordering of QWs has also been demonstrated for other impurity species, such as Si diffusion,\textsuperscript{2,1,1} and S diffusion.\textsuperscript{2,1,2} Ion-implantation has also been employed to enhance the disordering of QW structures. Implantation-induced disordering of QW structures has been demonstrated for various species implants, including Zn,\textsuperscript{2,1,3} Si,\textsuperscript{2,1,4} B and F\textsuperscript{2,1,5} implants.

Impurity-free vacancy diffusion also results in an enhanced interdiffusion process. The method uses native defects to produce enhanced intermixing of the group III atoms at the interface. SiO\textsubscript{2} (or SiN\textsubscript{x}) capping layers are deposited on selected areas of the QW structure. The enhanced intermixing is attributed to Ga atoms outdiffusing into the encapsulating SiO\textsubscript{2}, which has been shown to have a great affinity for Ga.\textsuperscript{2,1,6} Group III vacancies are thus created at the surface, and these vacancies then diffuse through the structure during a rapid thermal annealing process, enhancing the intermixing.\textsuperscript{2,1,7} The surface defects can alternatively be generated by shallow ion implantation and are then driven deeper into the QW structure during the rapid thermal anneal.\textsuperscript{2,1,8} Again the presence of these vacancies at the well-barrier interfaces enhances the anneal driven interdiffusion of the group III atoms. Disordering of both AlGaAs/GaAs, InGaAs/GaAs, and In\textsubscript{0.5}Ga\textsubscript{0.4}As/InP QW structures by impurity-free vacancy diffusion has been
The well widths of strained QWs must be sufficiently below the critical thicknesses to maintain a coherently strained structure after disordering.\textsuperscript{2,119}

The interdiffusion of the constituent atoms across the well-barrier interface leads to a transition from an as-grown square well compositional profile to a nonlinear graded profile, which can be described by an error function distribution,\textsuperscript{2,120} as shown in Fig. 2.15. This compositional modification in strained material systems raises the question of the QW quality after interdiffusion. It has been demonstrated that the FWHM of PL spectra of thermally annealed InGaAs/GaAs QWs show little broadening for QWs within the critical thickness regime, indicating that no degradation in the quality of the strained QW has taken place.\textsuperscript{2,105} In the case of Zn enhanced interdiffusion, some broadening of PL spectra occurred after disordering\textsuperscript{2,110} but the spectra indicated that the QWs were still coherently strained. InGaAs/GaAs single QWs disordered by shallow As implantation and thermal annealing also showed little broadening of PL peaks,\textsuperscript{2,119} while an early study reported that strained layer superlattices demonstrate good structural integrity after ion implantation.\textsuperscript{2,121} Investigation into Zn diffusion induced disordering of In\textsubscript{0.53}Ga\textsubscript{0.47}As/InP QWs, which results in a strained structure, also reported\textsuperscript{2,111} that high-resolution transmission electron microscopy lattice images of the disordered QW structure showed no misfit dislocations or microtwins, indicating that the disordered structure is coherently strained. With careful processing, coherently strained QW structures are possible even after disordering.

\textbf{2.6. Summary}

The lattice-mismatch in strained-layer structures can be accommodated by coherent strain if the strained layer is below a critical thickness. The strain induced in such a structure is influenced by the composition of the buffer layer between the structure
Fig. 2.15. Schematic conduction (C) and hole (V) band diagram of the error function profile quantum well structure.
and the substrate. Strain has three major effects on the band structure at the $\Gamma$ valley: modification of the bandgap energy between the conduction and valence bands, lifting of the HH and LH degeneracy, and the introduction of anisotropy in the hole effective masses. Square QW structures result in a series of discrete energy levels inside potential wells, and their position within the wells depends on the carrier confinement profiles, which in turn are influenced by the band offsets for the material system. QW structures offer a wider range of principal transition energies than that possible with bulk materials. Strained QW structures offer an extra degree of freedom in bandgap engineering.

Non-square confinement profiles have been investigated for increased flexibility in customising the optical properties of QW devices. Selective area disordering of QWs, which modifies a square QW into a nonlinear graded QW, is being widely studied as a post-growth technique for modifying optical properties in localised areas, leading to enhanced device performance and additionally making possible monolithic integration of optical and electronic devices. Significant advances have been made in the well-understood AlGaAs/GaAs material system. InGaAs/GaAs and In$_{0.35}$Ga$_{0.65}$As/InP disordered QW structures are also being actively investigated to enable similar developments in the performance of optical devices, and in monolithic integration of these devices, at longer wavelengths than those applicable to AlGaAs/GaAs. The design and analysis of these devices requires a knowledge of how the optical properties of the QW vary as a function of the extent of disordering. In the rest of this thesis the subband structure of strained, disordered InGaAs/GaAs single QWs is determined and the effects of strain and disordering on the absorption coefficient and refractive index, as well as on the exciton Stark shift and electroabsorption, are considered. The model developed is extended to In$_{0.35}$Ga$_{0.65}$As/InP single QWs which, starting as a lattice-matched QW, can become strained after disordering.
2.7. References


Chapter 2


Chapter 2


2.120. T.E. Schlesinger and T. Kuech, Appl. Phys. Lett. 49, 519 (1986).

Chapter 3

SUBBAND STRUCTURE OF A DISORDERED InGaAs/GaAs SINGLE QUANTUM WELL

Determination of the subband structure of InGaAs/GaAs quantum wells (QWs) requires the consideration of both strain and carrier confinement effects. For disordered InGaAs/GaAs QWs it is necessary to understand how the combined effects of disordering and strain modify the carrier confinement profiles in order to be able to determine the subband edge structure and the valence subband dispersion.

3.1. Introduction

The effects of thermal annealing on InGaAs/GaAs QW structures have been investigated using x-ray diffraction studies of strained-layer superlattices (SLSs), low temperature PL spectroscopy of SLSs and single QWs. The results reported were interpreted in terms of the interdiffusion of In and Ga atoms across the well-barrier interface, resulting in disordered QW structures. The thermally-driven interdiffusion is enhanced by impurity-induced disordering (IID) or impurity-free vacancy diffusion (IFVD). Enhancement of the compositional disordering by Zn diffusion, as well as by ion implantation of impurity species followed by thermal annealing, has been demonstrated in InGaAs/GaAs QWs. Disordering by Be, Zn, Si, and As implantation has been reported for selected sets of process conditions (implant energy, annealing temperature and time). Shallow As implantation followed by rapid thermal annealing has been used to demonstrate disordering by IFVD in InGaAs/GaAs...
QWs. The shift in peak positions of low temperature PL spectra was interpreted as arising from the interdiffusion of In and Ga, which is enhanced by diffusion of vacancies generated near the surface by the shallow ion implant. The disordering process modifies the as-grown square well compositional profile to a graded profile, altering the carrier confinement profile and subband structure in the QW. The extent of the QW shape modification in IID is found to depend on the type and concentration (dose) of the impurity (implanted) species, and the anneal temperature and time. In IFVD the extent of the interdiffusion depends on the anneal temperature and time, and the excess vacancy concentration.

The constituent atoms distribution after interdiffusion has been modelled by an error function profile. The error function distribution results from summing the effects of a series of line sources representing an extended source of limited extent, each yielding a Gaussian distribution, and assumes that the interdiffusion process across the well-barrier interface follows Fick’s second law of diffusion. Since the discovery of IID of QW structures various computational techniques have been used to investigate theoretically the subband states in the disordered QWs. Numerical results for the electron and heavy hole (HH) subband ground states in disordered AlGaAs/GaAs QWs using a variational calculation have been reported for an error function potential well. The electron and HH subband states for disordered AlGaAs/GaAs QWs were obtained for the error function distribution using a particle transmission calculation. The subband energies and wave functions for an error function compositional profile have also been calculated in the AlGaAs/GaAs material system taking into consideration a nonparabolic band model for the electron effective mass, and the valence subband mixing between the heavy and light holes. A Green’s function model and a hyperbolic function model have also been used to study theoretically the subband structure and optical
properties of disordered AlGaAs/GaAs single QWs. In the strained InGaAs/GaAs material system, calculations of the ground state only have been reported for disordered QWs, using a Green’s function approach for the compositional profile and a variational technique to obtain the ground state. In the study presented here the effects of strain and disordering on the carrier confinement profile are considered for an error function compositional distribution, and the energy and wave functions for all the subband states in disordered InGaAs/GaAs single QWs are determined by means of a finite difference method using the envelope function scheme with an effective mass approximation.

3.2. Subband Structure in the Envelope Function Approximation

3.2.1. Envelope Function Approximation

The quantum-mechanical wave function describing the physical state of the carrier in a QW structure is the sum of products of the rapidly varying periodic parts of the band edge Bloch functions for the bulk materials and slowly varying functions (on the scale of the host crystal unit cells) for the QW confinement, called the envelope functions, where the summation runs over the host band edges. Within the framework of the envelope function scheme, the expansion for the wave function is written as:

$$\Psi(k_\parallel, z) = e^{i\mathbf{k}_\parallel \cdot \mathbf{r}} \sum_n u_{n0}(\mathbf{r}) \chi_n(z)$$  \hspace{1cm} (1)$$

where $u_{n0}$ are the band edge Bloch functions, $\chi_n$ are the envelope functions, $z$ is the confinement (and growth) axis, $n$ is a bulk band index, $k_\parallel = (k_x, k_y)$ is the in-plane wave vector parallel to the plane of the QW layer, $\mathbf{r} = \mathbf{r}(x, y, z)$ and $\mathbf{r}_\parallel = \mathbf{r}(x, y)$ are position vectors.
The envelope function approximation takes advantage of two considerations. The first is that the host materials creating the QW structure display similar band structures, and that moreover, the periodic part of the Bloch functions of the relevant band edges do not differ very much from one host material to the other. The second arises from the fact that the relevant electronic states of the actual structure are often close to the band extrema of the hosts so that only a small fraction of the host Brillouin zone needs to be considered. The summation is therefore restricted to eight bands (which are, including spin degeneracy, the two conduction bands at \( \Gamma \), the upper four valence bands around \( \Gamma \), and the two split-off bands at \( \Gamma \), Fig. 2.4), or to six bands if the split-off bands are neglected. The rapidly varying terms will enter in the subsequent calculations only through effective parameters, which are assumed in the envelope function approximation to be known a priori. The envelope functions, which account for the band edge perturbation, are solutions to the relevant Schrödinger-like equation governing their spatial behaviour.

At the Brillouin zone centre, \( k_{||} = 0 \) (the \( \Gamma \) point), there is no heavy hole and light hole subband mixing. If in addition, the electron subbands are taken to be uncoupled from the hole subbands (and so are parabolic), the electron and hole quantized energy levels may be found by solving the respective one-dimensional Schrödinger equation for the envelope function \( \chi_{\alpha}(z) \), using the Ben Daniel and Duke model, with an effective mass approximation. The equation can be expressed as:

\[
-\frac{\hbar^2}{2 m_{\perp}(z)} \frac{d}{dz} \left[ \frac{1}{m_{\perp}(z)} \frac{d \chi_{\alpha}(z)}{dz} \right] + U(z) \chi_{\alpha}(z) = E_{\alpha} \chi_{\alpha}(z)
\]

where \( U(z) \) is the carrier confinement profile, given by the spatially-varying band edge energies of the semiconductor structure, \( E_{\alpha} \) is the quantized energy level with the
subband energy zero at the bottom of the QW, $m_{\perp}^*(z)$ is the spatially-varying band edge carrier effective mass in the $z$-direction, $r$ denotes either the electron (C), or heavy hole (V=HH), or light hole (V=LH), $\ell = p$ or $q$ refers to the quantized subband energy levels for the electrons and holes, respectively, and $\hbar$ is Planck's constant. Since a parabolic band approximation is assumed, the total energy of a subband state is

$$E_{\text{tot}} = E_{\text{envelope}} + \frac{\hbar^2 k_{||}^2}{2m_{||}^r},$$

where $m_{||}^r$ is the carrier effective mass in the plane of the QW.

For an undoped, as-grown QW a square spatial variation results in the $z$-direction, for the carrier effective mass and the carrier confinement profile, with a step at the well-barrier interface. In non-square QW structures a graded spatial variation has to be considered in determining the quantized energy levels and envelope wave functions.

When band mixing is taken into consideration the more general, multiband effective mass method can be applied to the QW problem, and has proved useful because of the insight it gives into valence subband mixing. The valence subband structure can be described by a multiband effective mass equation based on the $k \cdot p$ method of Luttinger-Kohn. This retains the three highest (doubly degenerate) valence bands, so that a $6 \times 6$ Luttinger-Kohn Hamiltonian results, with the off-diagonal terms in the Hamiltonian describing the dispersion of and interactions between the bands up to order $k^2$. If the spin-orbit splitting gap is large and interaction with the split-off band is neglected a $4 \times 4$ Hamiltonian is used.

### 3.2.2. Envelope Function Approximation in Strained-Layer Structures

The presence of strain in a QW leads to the splitting of the HH and LH bands at $k_{||} = 0$ and also induces coupling between the LH and spin-orbit bands. These
effects result in strain-dependent bandgaps that modify the carrier confinement profiles, $U_j(z)$. One approach used to determine the subband edge ($k_{||} = 0$) structure of strained square QWs is to introduce these modifications in eq. (2) which is then used to extract the subband energy levels and the wave functions.\textsuperscript{3,35,3,36} In a second approach, using the multiband effective mass method, the strain-dependent terms are included in the Luttinger-Kohn Hamiltonian.\textsuperscript{3,37} For an exact description of the valence subband dispersion of strained QWs it is necessary to retain the three highest (doubly degenerate) valence bands\textsuperscript{3,38,3,39} in order to account for the strain-induced coupling between the LH and spin-orbit bands. If the spin-orbit splitting and the bandgap energy are, however, large compared with the strain effect, the first method is a good approximation to the more exact second approach for calculations at $k_{||} = 0$.\textsuperscript{3,35,3,36}

For $k_{||} \neq 0$ the exact solution using the 6x6 Hamiltonian is quite complicated. As a first approximation, for small values of strain compared with the spin-orbit splitting, the split-off band can be ignored, returning to the 4x4 Hamiltonian,\textsuperscript{3,39} which can be solved using a finite difference method,\textsuperscript{3,37} or alternatively, by means of approximate methods that have been developed to obtain a solution in the neighbourhood of $k_{||} = 0$ for the valence subband dispersion.\textsuperscript{3,40,3,41} The approach used here is the one developed by Chan using an effective Hamiltonian,\textsuperscript{3,41} and is outlined in section 3.3.3. below.

\section*{3.3. Computational Considerations}

The theoretical considerations used to model the effects of strain and disordering on the carrier confinement profiles of undoped, pseudomorphic, disordered InGaAs/GaAs single QWs are described in this section, as well as the calculations used to arrive at the subband edge structure, and the subband structure for finite $k_{||}$, that result from these confinement profiles.
3.3.1. Effects of Strain and Disordering on the Carrier Confinement Profile

In lattice-mismatched quantum well heterostructures, the mismatch between the well and barrier materials is taken up by uniform elastic strain if the layers are sufficiently thin. In pseudomorphic strained-layer structures the in-plane lattice constant of the structure matches that of the substrate so that the QW layer accommodates all of the strain while the barrier layer is unstrained. Within the critical thickness regime, the QW lattice constant parallel to the interface matches the in-plane lattice constant by compression or expansion in the interfacial plane. A tetragonal deformation also takes place so that the QW layer is compressed or expanded in the direction perpendicular to the interface. The QW will be coherently strained with a biaxial hydrostatic strain parallel to the interfacial plane and a uniaxial shear strain perpendicular to the interfacial plane. A compressive (tensile) hydrostatic strain causes an increase (decrease) in the bandgap energy by an amount determined by the hydrostatic deformation potential, defined as the shift in energy of the band edge per unit hydrostatic strain. The uniaxial (shear) strain disrupts the cubic symmetry of the semiconductor and lifts the degeneracy of the HH and LH band edges at the Brillouin zone centre \( \Gamma \). The heavy hole band moves towards (away from) the conduction band and the light hole band moves away from (towards) the conduction band. In addition, the presence of strain induces coupling between the LH valence band and the split-off band.

The carrier confinement profiles for electron, HH and LH in the as-grown \( \text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs} \) system have a square shape whose depth is dependent on the In content \( x \), the offset ratio, and on the effects of strain outlined above, and each supports a number of quantized energy levels. Since the strain in the InGaAs layer is compressive the HH confinement potential well depth is larger than that of the LH potential well.
The disordering process in InGaAs/GaAs QW structures results in the interdiffusion of Group III (In and Ga) atoms across the well-barrier interface. The interdiffusion is characterized by a diffusion length \( L_d \), which is defined here as

\[
L_d = (Dt)^{1/4},
\]

where \( D \) is the diffusion coefficient and \( t \) is the processing time. A small \( L_d \) corresponds to the initial stages of disordering with the QW compositional profile remaining almost rectangular, while a larger \( L_d \) corresponds to a more extensively disordered QW structure.

After interdiffusion, the In concentration, \( \bar{x}(z) \), across the InGaAs/GaAs QW structure is assumed to have an error function profile, given by:

\[
\bar{x}(z) = \frac{x}{2} \left[ \text{erf} \left( \frac{L_z + 2z}{4L_d} \right) + \text{erf} \left( \frac{L_z - 2z}{4L_d} \right) \right]^{1/2}
\]

where \( z \) is the growth direction, \( L_z \) is the well width, with the QW centred at \( z = 0 \). The compositional profile in the QW structure after interdiffusion implies that the carrier effective mass in the \( z \) direction, the bulk bandgap, and the hydrostatic and shear strain vary continuously across the QW.

Consequently, the spatial variation in the \( z \)-direction of the carrier effective mass, \( m^{*}_{zz}(\bar{x}) \), is now obtained from \( m^{*}_{zz}(\bar{x}) = m^{*}_{xx}(x=\bar{x}(z)) \), where \( m^{*}_{xx}(x) \) is the carrier bulk effective mass.

The unstrained bandgap in the well, \( E_g(x) \), is also a function of the compositional profile, so that the unstrained potential profile after interdiffusion, \( \Delta E_g(\bar{x}) \), varies across the well and is given by:

\[
\Delta E_g(\bar{x}) = Q_e \Delta E_g(x=\bar{x})
\]

where \( Q_e \) is the band offset ratio and \( \Delta E_g \) is the unstrained bandgap offset.

The in-plane strain across the well, \( \epsilon(\bar{x}) \), will also vary so that the strain effects are also \( z \)-dependent. Assuming that the growth direction \( z \) is along \(<001>\), then for the
biaxial stress parallel to the interface the strain components, after interdiffusion, are given by:\textsuperscript{3,44}

\[\begin{align*}
\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon(\bar{x}) \\
\varepsilon_{zz} &= -2[c_{12}(\bar{x})/c_{11}(\bar{x})] \varepsilon(\bar{x}) \\
\varepsilon_{xy} &= \varepsilon_{yx} = \varepsilon_{zx} = 0
\end{align*}\]

where \(\varepsilon(\bar{x})\) is defined to be negative for compressive strain, and \(c_i(\bar{x})\) are the elastic stiffness constants.

The change in the bulk bandgap, \(S_1(\bar{x})\), due to the biaxial component of strain is given by:\textsuperscript{3,44}

\[S_1(\bar{x}) = -2a(\bar{x})[1 - c_{12}(\bar{x})/c_{11}(\bar{x})] \varepsilon(\bar{x})\]

where \(a(\bar{x})\) is the hydrostatic deformation potential calculated from:\textsuperscript{3,44}

\[a(\bar{x}) = -\frac{3}{\varepsilon} [c_{11}(\bar{x}) + 2c_{12}(\bar{x})] \frac{dE_g}{d\bar{P}}(\bar{x})\]

where \(dE_g/d\bar{P}\) is the hydrostatic pressure coefficient of the lowest direct energy gap \(E_g\).

The splitting energy, \(S_{||}(\bar{x})\), between the HH and LH band edges induced by the uniaxial component of strain is given by:\textsuperscript{3,44}

\[S_{||}(\bar{x}) = -b(\bar{x})[1 + 2c_{12}(\bar{x})/c_{11}(\bar{x})] \varepsilon(\bar{x})\]

where \(b(\bar{x})\) is the shear deformation potential. The parameters \(a, b, c_{ij}, dE_g/d\bar{P}\) in eq. (6) to (9) above are assumed to obey Vegard's law:\textsuperscript{3,44,46} so that their respective values depend directly on the compositional profiles across the QW.

In the case of InGaAs/GaAs it is assumed that the LH and spin-orbit bands are coupled due to the presence of the stress while the HH state remains uncoupled.\textsuperscript{3,34} The valence band splitting at \(k_{||} = 0\) for the HH band and for the LH band (which includes mixing with the split-off band) are then given by:\textsuperscript{3,33,38}

\[S_{HHe}(\bar{x}) = S_{||}(\bar{x})\]
\[ S_{\text{HH},\text{LH}}( \bar{x} ) = -\frac{1}{2} [ S_{\text{HH}}( \bar{x} ) + \Delta_s( \bar{x} )] + \frac{1}{2} [9 \{ S_{\text{HH}}( \bar{x} ) \}^2 + \{ \Delta_s( \bar{x} ) \}^2 - 2 S_{\text{HH}}( \bar{x} ) \Delta_s( \bar{x} )]^{1/2} \]  

(11)

respectively, where \( \Delta_s( \bar{x} ) \) is the spin-orbit splitting.

The QW confinement potential after the disordering process, \( U_f(z) \), is obtained by modifying the unstrained potential profile after processing, \( \Delta E_f(\bar{x}) \), by the variable strain effects, and is given by:

\[ U_f(z) = \Delta E_f(\bar{x}) - S_{\text{ff}}(\bar{x}) \pm S_{\text{ff}}(\bar{x}) \]  

(12)

where \( S_{\text{ff}}(\bar{x}) = Q_f S_f(\bar{x}) \), the '-' and '+' signs represent the confined HH and LH profiles, respectively, and \( S_{\text{ff}}(\bar{x}) = 0 \).

Thus, due to the presence of strain different confinement potential profiles result for the HH and LH (as well as spin-orbit) bands, while disordering produces non-square, graded profiles, see Fig. 3.1. Since the hole occupancy of the spin-orbit split-off band is negligibly small,\(^3\,47\) the details of its subband structure are not considered here.

### 3.3.2. Subband Edge Calculation

The subband structure at \( k_{||} = 0 \) for the disordered InGaAs/GaAs QW is determined by solving the Schrödinger eq. (2) above, using eq. (12) for the carrier confinement profile, \( U_f(z) \). The Schrödinger equation is solved numerically, using a finite difference method, to obtain the quantized energy levels, \( E_{\text{cp}}, E_{\text{vq}} \), and the envelope wave functions \( \chi_{\text{cp}}, \chi_{\text{vq}} \). The equation is discretised into a non-uniform finite difference grid and the eigenvalues obtained using a bisection method. These bound states are determined by solving the graded QW within a QW with infinitely high barriers so that the long range behaviour of the envelope function is specified by the boundary condition \( \chi_f(\pm z_b) = 0 \), where \( z_b \) is very large compared to the well width, approximating the thick barrier. A value of \( z_b = 500 \text{ nm} \) is used in the numerical calculations.
Fig. 3.1. Schematic diagram showing the effects of strain and disordering on the carrier confinement profiles in a disordered In$_{0.2}$As$_{0.8}$As/GaAs single QW, for $L_d = 1.5$ nm. The dashed lines represent the unstrained bandgap after disordering, and the dot-dash line shows how the unstrained bandgap is modified by the effect of the hydrostatic strain. The solid line represents the final electron (C), HH and LH confinement profile. Note that for the electron confinement profile, the dot-dash and solid lines coincide. All terms are with reference to the centre of the well, $z = 0$. 
The electron-heavy hole transition energy, $E_{CpHq}$, and the electron-light hole transition energy, $E_{CpLq}$, can then be obtained from

$$E_{CpHq} = E_{BHH}(x(0)) + E_{Cp} + E_{BHQ}$$

$$E_{CpLq} = E_{BHLH}(x(0)) + E_{Cp} + E_{LHQ}$$

respectively, where $E_{BHH}(x(0))$, $E_{BHLH}(x(0))$ are the electron-heavy hole and electron-light hole lowest direct bandgap at the $\Gamma$ point after disordering, respectively (see Fig. 3.1).

The overlap integral $<X_{Cp}|X_{Vq}>$ between the $p$th conduction subband and the $q$th valence subband envelope functions, is calculated using

$$<X_{Cp}|X_{Vq}> = \int_{z_l}^{z_b} X_{Cp}^*(z)X_{Vq}(z) \, dz$$

$|<X_{Cp}|X_{Vq}>|^2$ is a measure of the interband transition selection rule.

### 3.3.3. Subband Structure Calculation

In a QW structure, the envelope function associated with each hole subband varies with $k_{||}$ because of the coupling of subbands. This valence-band coupling mixes the LH and HH subbands away from $k_{||} = 0$ and generates nonparabolicities in the hole subband structure which change the effective in-plane masses. The valence subband dispersion for the disordered InGaAs/GaAs QW is obtained here by using an effective Hamiltonian approach, briefly outlined below.

The coupled envelope function $\chi_{V}(k_{||}, z)$ of a hole subband at any finite $k_{||}$ not too far away from the highest symmetry point ($k_{||} = 0$), can be written as a linear combination of the decoupled $z$-direction envelope functions $\chi_{V}(z)$ of all hole subbands at $k_{||} = 0$, which are obtained $a \text{ priori}$ from the solution of eq. (2). Since only a finite dimension basis set for the expansion is used in practice, the approximation is used for
a limited range of \( k \). The expression of the envelope function at finite \( k_{\parallel} \) is defined as follows:

\[
\chi_{\nu}(k_{\parallel}, z) = \sum_{q=1}^{N} \sum_{\nu = -3/2}^{3/2} A_{\nu,q}(k_{\parallel}) \chi_{\nu,q}(z)
\]

where \( \nu \) runs over the fourfold degenerate hole states and \( N \) is the maximum number of basis taken in each \( \nu \). With this basis the effective Hamiltonian is:

\[
\begin{bmatrix}
E_{3/2} & C & B & 0 \\
C^* & E_{1/2} & 0 & B^* \\
B^* & 0 & E_{3/2} & C^* \\
0 & B^* & C^* & E_{3/2}
\end{bmatrix}
\]

where

\[
C_{qd} = \sqrt{3} \frac{\hbar^2}{2m_0} \gamma_2 (k_x - ik_y) \int_0^{z_0} \chi_{3/2,q}(z) \chi_{1/2,q}(z) \, dz
\]

\[
B_{qd} = \sqrt{3} \frac{\hbar^2}{m_0} \gamma_2 (-k_x - ik_y) \int_0^{z_0} \chi_{3/2,q}(z) \frac{d}{dz} \chi_{1/2,q}(z) \, dz
\]

\[
E_{\pm 3/2, ss'} = \delta_{ss'} E_{HH} - \frac{\hbar^2}{2m_{\parallel}^*} k_{\parallel}^2
\]

\[
E_{\pm 1/2, ss'} = \delta_{ss'} E_{HL} - \frac{\hbar^2}{2m_{\parallel}^*} k_{\parallel}^2
\]

where \( \delta_{ss'} E_{HH} = E_{g}(\tilde{x}(0)) - S_{\perp}(\tilde{x}(0)) + S_{\parallel\parallel}(\tilde{x}(0)) \), \( \delta_{ss'} E_{HL} = E_{g}(\tilde{x}(0)) - S_{\perp}(\tilde{x}(0)) - S_{\parallel\perp}(\tilde{x}(0)) \), \( \gamma_2 \) is the Luttinger-Kohn parameter,\(^3\)\(^4\) \( m_{\parallel}^* \) is the hole effective mass in the plane of the QW, and \( 2 z_k \) is the width of a square QW with infinitely high barrier which contains the disordered QW. The introduction of this larger well is to numerically determine the continuum levels above the top of the disordered QW.
3.4. Results and Discussion

In order to investigate the effect of strain and disordering on the confinement profile and the HH-LH band edge splitting, and determine the subband structure, an undoped 10 nm thick In$_{0.2}$Ga$_{0.8}$As layer sandwiched between thick GaAs barriers is considered, and results obtained for the disordered structure for various stages of interdiffusion. The QW structure is assumed to be pseudomorphic so that the InGaAs layer is compressively strained while the GaAs barrier is unstrained. The thickness of the QW is within the critical layer thickness requirements for the particular strained-layer system.$^{3,43}$ Table 3.1 lists relevant material parameters used in the numerical calculations.

3.4.1. Subband Edge Structure

The In concentration after interdiffusion is described by the error function profile. When interdiffusion starts ($L_d = 1$ nm approximately) the In atoms move into the barrier while at the centre of the well the In concentration remains unchanged. However, subsequent interdiffusion rapidly reduces the In concentration at the well centre as the In atoms diffuse deeper into the barrier, tending towards a uniform distribution across the structure. The resulting graded compositional profile modifies the strain profile in the QW, as shown in Fig. 3.2. In the as-grown ($L_d = 0$) structure, the strain in the well is constant, while for the disordered structures ($L_d = 1$ and 4 nm), the strain across the well varies, with a maximum strain at the centre of the well. Thus the increase in the bandgap energy caused by the hydrostatic compressive strain is greatest at the well centre and decreases to zero away from the well centre. This can be seen in Fig. 3.1 where, for the conduction band, the effect of the hydrostatic component of the strain, $Q_c S_d(x)$, is represented by the gap between the dashed and the solid profiles.
**Table 3.1.**

Parameters used in the numerical calculations for $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ single QW structure. $a_0$ is the lattice constant, $m_0$ is the electron mass in free space.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\text{In}<em>x\text{Ga}</em>{1-x}\text{As}$</th>
<th>Units</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>$5.6533 + 0.4051x$</td>
<td>Å</td>
<td>3.46</td>
</tr>
<tr>
<td>$c_{11}$</td>
<td>$11.88 - 3.55x$</td>
<td>$10^{11}$ dyn/cm$^2$</td>
<td>3.46</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>$5.38 - 0.854x$</td>
<td>$10^{11}$ dyn/cm$^2$</td>
<td>3.46</td>
</tr>
<tr>
<td>$dE_g/dP$</td>
<td>$11.5 - 1.5x$</td>
<td>$10^{-6}$ eV/bar</td>
<td>3.46</td>
</tr>
<tr>
<td>$b$</td>
<td>$-1.7 - 0.1x$</td>
<td>eV</td>
<td>3.46</td>
</tr>
<tr>
<td>$m_c^*$</td>
<td>$0.067 - 0.044x$</td>
<td>$m_0$</td>
<td>3.49</td>
</tr>
<tr>
<td>$m_{\perp\text{HH}}^*$</td>
<td>$0.340 - 0.070x$</td>
<td>$m_0$</td>
<td>3.49</td>
</tr>
<tr>
<td>$m_{\perp\text{LH}}^*$</td>
<td>$0.087 - 0.062x$</td>
<td>$m_0$</td>
<td>3.49</td>
</tr>
<tr>
<td>$m_{\parallel\text{HH}}^*$</td>
<td>$0.11 - 0.075x$</td>
<td>$m_0$</td>
<td>3.50</td>
</tr>
<tr>
<td>$m_{\parallel\text{LH}}^*$</td>
<td>$0.21 - 0.120x$</td>
<td>$m_0$</td>
<td>3.50</td>
</tr>
<tr>
<td>$E_g$</td>
<td>$1.424 - 1.53x + 0.45x^2$</td>
<td>eV</td>
<td>3.49</td>
</tr>
<tr>
<td>$\Lambda_0$</td>
<td>$0.341 - 0.09x + 0.14x^2$</td>
<td>eV</td>
<td>3.51</td>
</tr>
<tr>
<td>$Q_c/Q_V$</td>
<td>70:30</td>
<td></td>
<td>3.49</td>
</tr>
</tbody>
</table>

68
Fig. 3.2. In-plane strain across the disordered QW for various values of \( L_d \). \( L_d = 0 \) nm (solid line), \( L_d = 1 \) nm (dashed line), \( L_d = 4 \) nm (dotted dash line).
while for the valence band, the effect of the hydrostatic component of the strain, \( Q_V S_1(\bar{x}) \), is represented by the gap between the dashed and the dot-dashed profiles. The uniaxial strain follows a similar profile as the in-plane strain, so that the HH-LH splitting effect of the uniaxial strain is greatest at the well centre, decreasing to zero away from the well centre. This is also illustrated in Fig. 3.1, where the effect of the uniaxial strain on the HH and LH confinement profile, \( S_{1\text{HH}}(\bar{x}) \) and \( S_{1\text{LH}}(\bar{x}) \), respectively, is represented by the gap between the dot-dashed and the solid profiles. The effect of the strain-induced coupling between the LH and spin-orbit bands can be seen from the fact that the magnitudes of \( S_{1\text{HH}}(\bar{x}) \) and \( S_{1\text{LH}}(\bar{x}) \) are not equal, with \( S_{1\text{LH}}(\bar{x}) \) being less than \( S_{1\text{HH}}(\bar{x}) \).

The effects of strain on the disordered QW are therefore reflected in both the maximum depth, \( U(z=0) \), and the shape of the carrier confinement profiles. By altering the C-HH bandgap and the C-LH bandgap, the compressive strain effectively increases (decreases) the depth of the HH (LH) confinement wells. Starting with a band offset ratio \( Q_{C}\)-\( Q_V \) of 70:30 for the InGaAs/GaAs material system, the presence of strain results in an effective offset ratio \( Q'_{C}:Q'_{HH} \) of 55:45 and an effective offset ratio \( Q'_{C}:Q'_{LH} \) of 87:13 in the as-grown QW considered here, where the effective offset ratio \( Q'_{C} \) is the ratio of the maximum depth of the carrier confinement profile to the maximum bandgap offset of the strained QW. The LH confinement potential depth is thus considerably smaller than the HH confinement potential depth.

The subband edge energy levels, for different values of \( L_d \), together with the corresponding values of the as-grown QW (equivalent to \( L_d = 0 \)) are given in Table 3.2. Similar results for \( L_d = 50 \) nm are presented in Table 3.3. Fig. 3.3 shows the electron (C), and HH confinement profiles and ground states for the as-grown, and disordered QW for various values of \( L_d \). As the interdiffusion proceeds the depth of the
Table 3.2.
The subband energy levels for the interdiffused QW for various values of $L_d$ (nm). The energy values are taken positively from the zero potential of the respective QW.

<table>
<thead>
<tr>
<th>Subband Level</th>
<th>Subband-Level Energy (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$L_d = 0$</td>
</tr>
<tr>
<td>C1</td>
<td>27.75</td>
</tr>
<tr>
<td>C2</td>
<td>98.85</td>
</tr>
<tr>
<td>C3</td>
<td>--</td>
</tr>
<tr>
<td>C4</td>
<td>--</td>
</tr>
<tr>
<td>HH1</td>
<td>7.66</td>
</tr>
<tr>
<td>HH2</td>
<td>30.15</td>
</tr>
<tr>
<td>HH3</td>
<td>65.32</td>
</tr>
<tr>
<td>HH4</td>
<td>--</td>
</tr>
<tr>
<td>HH5</td>
<td>--</td>
</tr>
<tr>
<td>HH6</td>
<td>--</td>
</tr>
<tr>
<td>HH7</td>
<td>--</td>
</tr>
<tr>
<td>LH1</td>
<td>9.82</td>
</tr>
</tbody>
</table>

Table 3.3.
Subband energy levels for $L_d = 50$ nm.

<table>
<thead>
<tr>
<th>Level</th>
<th>Subband Energy (meV)</th>
<th>Level</th>
<th>Subband Energy (meV)</th>
<th>Level</th>
<th>Subband Energy (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.597</td>
<td>HH1</td>
<td>0.244</td>
<td>HH10</td>
<td>3.887</td>
</tr>
<tr>
<td>C2</td>
<td>1.746</td>
<td>HH2</td>
<td>0.723</td>
<td>HH11</td>
<td>4.189</td>
</tr>
<tr>
<td>C3</td>
<td>2.802</td>
<td>HH3</td>
<td>1.185</td>
<td>HH12</td>
<td>4.468</td>
</tr>
<tr>
<td>C4</td>
<td>3.762</td>
<td>HH4</td>
<td>1.629</td>
<td>HH13</td>
<td>4.720</td>
</tr>
<tr>
<td>C5</td>
<td>4.616</td>
<td>HH5</td>
<td>2.054</td>
<td>HH14</td>
<td>4.945</td>
</tr>
<tr>
<td>C6</td>
<td>5.356</td>
<td>HH6</td>
<td>2.461</td>
<td>HH15</td>
<td>5.140</td>
</tr>
<tr>
<td>C7</td>
<td>5.968</td>
<td>HH7</td>
<td>2.848</td>
<td>HH16</td>
<td>5.301</td>
</tr>
<tr>
<td>C8</td>
<td>6.437</td>
<td>HH8</td>
<td>3.216</td>
<td>HH17</td>
<td>5.428</td>
</tr>
<tr>
<td>LH1</td>
<td>0.101</td>
<td>LH2</td>
<td>0.261</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Fig. 3.3. Electron (C) and heavy hole (HH) confinement profiles for a single, undoped In$_{0.2}$Ga$_{0.8}$As/GaAs QW with $L_z = 10$ nm, for a range of diffusion lengths: $L_d = 0$ nm (solid line), $L_d = 1$ nm (dashed line), $L_d = 4$ nm (dotted dash line), $L_d = 8$ nm (dotted line). The ground states are also shown. The cross over points (COP) for electron confinement profiles are indicated.
confinement profile diminishes as the In profile changes shape, while the number of subband edge states increases. This can be explained in terms of a cross-over point (COP),\(^{3,24}\) which is defined as the potential, measured from the bottom of the disordered QW at \(z = \pm \frac{3}{2} L_d\). Below the COP, the width of the interdiffused well is smaller than the as-grown well width, so that the quantized energy levels in the interdiffused well shift upwards from the square QW levels; above the COP the well width is larger so that the energy levels in the interdiffused well shift downwards and more levels are supported. Thus inspection of the Cl and HH1 levels in Table 3.2 and the relevant COP values, given in Table 3.4, for the various \(L_d\) stages shows that the energy levels in the disordered QW are lower than the corresponding square QW levels for \(L_d = 8\) nm since they lie above the COP, while for \(L_d = 1\) nm they are higher since they lie below the COP. From Table 3.4 it can be seen that as \(L_d\) increases, the COP moves nearer the well bottom and the disordered well is wider over a larger depth, so that more bound states exist. The change in COP (%) with increasing \(L_d\), for conduction, HH, and LH confinement profiles is shown in Fig. 3.4, where COP (%) is defined as:

---

**Table 3.4.**

Variation in QW parameters for different diffusion stages. Values of \(L_d\) in nm.

<table>
<thead>
<tr>
<th>(L_d = 0)</th>
<th>(L_d = 1)</th>
<th>(L_d = 4)</th>
<th>(L_d = 8)</th>
<th>(L_d = 50)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Delta E_C) (meV)</td>
<td>116.2</td>
<td>116.18</td>
<td>73.11</td>
<td>40.31</td>
</tr>
<tr>
<td>(\Delta E_{TH}) (meV)</td>
<td>96.78</td>
<td>96.74</td>
<td>60.47</td>
<td>33.19</td>
</tr>
<tr>
<td>(\Delta E_{LH}) (meV)</td>
<td>17.72</td>
<td>17.71</td>
<td>7.70</td>
<td>2.94</td>
</tr>
<tr>
<td>(COP_C) (meV)</td>
<td>--</td>
<td>57.35</td>
<td>18.77</td>
<td>3.50</td>
</tr>
<tr>
<td>(COP_{HH}) (meV)</td>
<td>--</td>
<td>48.19</td>
<td>15.65</td>
<td>2.90</td>
</tr>
<tr>
<td>(COP_{LH}) (meV)</td>
<td>--</td>
<td>12.37</td>
<td>3.01</td>
<td>0.37</td>
</tr>
<tr>
<td>(x(z=0))</td>
<td>0.2</td>
<td>0.1999</td>
<td>0.1246</td>
<td>0.0683</td>
</tr>
</tbody>
</table>
It can be seen that because of the strain present in the QW structure the COP (%) for the LH subband is markedly higher than that for the HH subband. The results presented in Table 3.3 for \( L_d = 50 \text{ nm} \), together with the corresponding very low COP (%), Table 3.4, show that for significantly high \( L_d \) a large number of levels are packed very closely into a very shallow and wide potential well just below the bandgap of bulk GaAs. The relatively high density of the confined states in the shallow well indicates a practically fully diffused and bulk-like material with a bandgap energy just below the barrier bulk band gap energy. Table 3.5 shows the increase in the number of subband levels as \( L_d \) increases, for the structure considered here. Note the minimum number of LH levels supported, which again reflects the small LH confinement profile depth caused by the compressive strain.

**Table 3.5.**

*Number of subband energy levels (C = electrons, HH = heavy holes, LH = light holes) for various values of \( L_d \), for In_{0.2}Ga_{0.8}As/GaAs single QW with \( L_z = 10 \text{ nm} \).*

<table>
<thead>
<tr>
<th>( L_d ) (nm)</th>
<th>0</th>
<th>1</th>
<th>4</th>
<th>8</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>HH</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>7</td>
<td>17</td>
</tr>
<tr>
<td>LH</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
Fig. 3.4. The change in COP (%) with increasing $L_d$, for conduction (C), heavy hole (HH), and light hole (LH) confinement profiles.
The envelope wave functions are also affected by the modified confinement profile. Two corresponding normalised wave functions for a square QW and a disordered QW are shown in Fig. 3.5, which show that the wave functions in the disordered QW are not as strongly confined as in the square QW. The wave functions spread out due to the widening of the well, and the probability for the confined carriers is larger near the well-barrier interface and lower at the centre of the well due to the effective mass variation across the QW. These results are similar to those reported in a trapezoidal QW, and parabolic QW.

The interband transitions energy at \( k_{||} = 0 \), and the corresponding values of \( |\langle \chi_{cp} | \chi_{vq} \rangle |^2 \), the square of the electron-hole wave function overlap, the overlap integral, for various values of \( L_d \) are shown in Table 3.6. In the case of the square QW the value of \( |\langle \chi_{cp} | \chi_{vq} \rangle |^2 \) of the off-diagonal transitions is much smaller than that of the diagonal transitions. This reflects the selection rule for dipole transitions between electron (level \( p \)) and hole (level \( q \)) subbands. The origin of the selection rule \( p = q \) \( (\Delta \ell = p - q = 0) \) arises from the near orthogonality of the electron and hole envelope wave functions. In the infinite square well approximation \( \chi_c \) and \( \chi_v \) are usually orthogonal, i.e. their overlap integral is zero unless they have equal quantum numbers. For finite square QWs, the wave functions are no longer exactly orthogonal as the presence of the wave function in the barrier depends on the quantum number. This leads to a relaxed selection rule \( (p + q = \text{even}) \) so that weak off-diagonal transitions may ensue. In the disordered QW the wave functions are quite different (Fig. 3.5), as noted above, so that the orthogonality is not so rigid leading to stronger off-diagonal overlapping wave functions, and thus relaxation of the selection rule is more evident.

The off-diagonal values of \( |\langle \chi_{cp} | \chi_{vq} \rangle |^2 \) increase as the potential profile moves from the square QW profile. Then as the interdiffusion process advances, the values
Fig. 3.5. Normalised $\chi^2$ for C1 and HH3 subband states for the as-grown ($L_z = 10$ nm, $L_d = 0$ nm), and disordered ($L_d = 4$ nm) QW.
Table 3.6.

Interband transitions energy and square of the overlap integral, $|\langle \chi_{cp} | \chi_{nu} \rangle|^2$. Values of $L_u$ in nm.

<table>
<thead>
<tr>
<th></th>
<th>$L_u = 0$</th>
<th>$L_u = 1$</th>
<th>$L_u = 4$</th>
<th>$L_u = 8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-HH1</td>
<td>1.2464</td>
<td>1.2542</td>
<td>1.3192</td>
<td>1.3625</td>
</tr>
<tr>
<td>C1-HH3</td>
<td>1.3041</td>
<td>1.3141</td>
<td>1.3491</td>
<td>1.3754</td>
</tr>
<tr>
<td>C1-HH5</td>
<td>--</td>
<td>--</td>
<td>1.3681</td>
<td>1.3853</td>
</tr>
<tr>
<td>C1-HH7</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.3914</td>
</tr>
<tr>
<td>C2-HH2</td>
<td>1.3400</td>
<td>1.3506</td>
<td>1.3696</td>
<td>1.3845</td>
</tr>
<tr>
<td>C2-HH4</td>
<td>--</td>
<td>1.4075</td>
<td>1.3946</td>
<td>1.3959</td>
</tr>
<tr>
<td>C2-HH6</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4041</td>
</tr>
<tr>
<td>C3-HH1</td>
<td>--</td>
<td>--</td>
<td>1.3716</td>
<td>1.3888</td>
</tr>
<tr>
<td>C3-HH3</td>
<td>--</td>
<td>--</td>
<td>1.4015</td>
<td>1.4017</td>
</tr>
<tr>
<td>C3-HH5</td>
<td>--</td>
<td>--</td>
<td>1.4205</td>
<td>1.4116</td>
</tr>
<tr>
<td>C3-HH7</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4177</td>
</tr>
<tr>
<td>C4-HH2</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4011</td>
</tr>
<tr>
<td>C4-HH4</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4125</td>
</tr>
<tr>
<td>C4-HH6</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4207</td>
</tr>
<tr>
<td>C1-LH1</td>
<td>1.3276</td>
<td>1.3333</td>
<td>1.3685</td>
<td>1.3910</td>
</tr>
<tr>
<td>C3-LH1</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>1.4173</td>
</tr>
</tbody>
</table>

$|\langle \chi_{cp} | \chi_{nu} \rangle|^2$

$L_u = 0$ | $L_u = 1$ | $L_u = 4$ | $L_u = 8$

0.9533 | 0.9301 | 0.9145 | 0.9232
0.0264 | 0.0591 | 0.0817 | 0.0722
--     | --     | 0.0036 | 0.0045
--     | --     | --     | 0.0000
0.6956 | 0.6338 | 0.6881 | 0.7470
--     | 0.3520 | 0.2793 | 0.2223
--     | --     | 0.0213 | 0.0304
--     | --     | 0.1408 | 0.4081
--     | --     | 0.4061 | 0.4009
--     | --     | --     | 0.1403
--     | --     | --     | 0.0305
--     | --     | --     | 0.0254
--     | --     | --     | 0.1673
0.8496 | 0.8265 | 0.7728 | 0.7449
--     | --     | --     | 0.2230
Fig. 3.6. Variation with $L_d$ of the square of the overlap integral, $|<\chi_{CP}|\chi_{Vq}>|^2$, for the C1–HH1 diagonal transition, and the C1–HH3 off–diagonal transition.
peak and start to decrease. The specific case of the variation with $L_d$ of $|\langle \chi_{cp} | \chi_{vq} \rangle |^2$ for the C1-HH3 transition is plotted in Fig. 3.6. It can be seen that as $L_d$ increases quite significantly the values of $|\langle \chi_{cp} | \chi_{vq} \rangle |^2$ tend to the original square QW values. This implies that the selection rule is once again more rigid, reflecting the fact that for sufficiently large $L_d$ the potential well profile returns towards a square QW profile which is now, however, very shallow and wide, and which supports densely packed subband states.

The values of $|\langle \chi_{cp} | \chi_{vq} \rangle |^2$ of the diagonal transitions follow a reverse variation, decreasing as the interdiffusion starts, dropping to a minimum and then increasing again as the interdiffusion proceeds further, Fig. 3.6 for C1-HH1 transition. These variations of $|\langle \chi_{cp} | \chi_{vq} \rangle |^2$ are similar to those reported in a square QW under an external electric field. Consequently, an optimal interdiffusion stage may be found for a more favourable off-diagonal transition.

The change in the in-plane strain (at the well centre) with increasing $L_d$, and the variation of ground state transition energy for electron-heavy hole (C1-HH1) and electron-light hole (C1-LH1) transitions with increasing interdiffusion are shown in Fig. 3.7. The compressive strain in the well is a maximum when $L_d = 0$ and decreases with increasing $L_d$. The ground state transition which dominates is the C1-HH1 transition and is a result of the compressive nature of the strain. As $L_d$ increases, the ground state transition energy increases, as evidenced in experimental results. The change in C1-HH1 transition energy in going from $L_d = 0$ to $L_d = 10$ nm corresponds to a blue shift in the wavelength of about 90 nm. Thus the absorption edge of the disordered QW structure is shifted to shorter wavelengths. From Fig. 3.7(b), it can be seen that the difference between C1-HH1 and C1-LH1 transition energies decreases with increasing
Fig. 3.7. Variation of (a) in-plane strain, and (b) ground state transition energy, with $L_d$. 
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with the effect that disordering reduces the polarization sensitivity of the InGaAs/GaAs QW. \(^3\)^56

Fig. 3.8 shows the variation of the C1-HH1 transition energy with both well width and indium content for various values of \(L_d\). The C1-HH1 transition energy is more sensitive to the indium content variation than to the well width variation. The transition energy change from \(L_d = 0\) to 8 nm for \(L_z = 5\) nm is almost the same as that for \(L_z = 10\) nm, Fig. 3.8(a). From Fig. 3.8(b), it can be seen that the higher the indium content, the larger is the possible transition energy variation with interdiffusion. These results show that the carrier confinement profile of disordered InGaAs/GaAs QWs is more sensitive to the indium content than to the well width of the as-grown QW. This indicates that in seeking to tailor the transition energy by disordering, it would be more favourable to start with an as grown \(\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}\) QW structure having as high a value of \(x\) as possible. The penalty would be a smaller well width, in order to maintain a coherently strained structure, although the ground state transition energy variation with disordering is larger for a QW structure with a large \(x\) and small \(L_z\) in contrast to one with a small \(x\) and large \(L_z\).

The HH-LH band edge splitting, caused by the uniaxial component of strain, is also affected by disordering. The variation of the HH-LH band edge splitting, at the well centre, with \(L_d\) is shown in Fig. 3.9(a) for \(x = 0.10\) and \(x = 0.20\). The splitting is maximum for the as-grown QW. In the initial stages of disordering (\(L_d \leq 1\) nm approximately) it does not change as the indium content, and thus the in-plane strain, at the well centre remains unchanged. As interdiffusion proceeds, however, the strain at the well centre decreases rapidly so that the HH-LH band edge splitting also decreases rapidly. Beyond \(L_d \approx 8\) nm the splitting decreases further but much more slowly. It can be seen that a much larger variation in the HH-LH band edge splitting results for the
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(i): $L_d = 0 \text{ nm}$; (ii): $L_d = 4 \text{ nm}$; (iii): $L_d = 8 \text{ nm}$

$x = 0.20$

**Fig. 3.8(a).** Variation of C1-HH1 transition energy with well width for three different values of $L_d$. 

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Fig. 3.8(b). Variation of C1-HH1 transition energy with indium content for three different $L_d$ values. The as-grown well width is $L_z = 10$ nm.
Fig. 3.9(a). Variation of the strain-induced HH-LH band edge splitting at the well centre with $L_d$, for two values of indium content.
Fig. 3.9(b). Variation of the strain-induced HH-LH band edge splitting at the well centre with as-grown well width, for three different values of $L_d$. 

(i): $L_d = 0$ nm;  (ii): $L_d = 2$ nm; (iii): $L_d = 4$ nm

$x = 0.20$
Fig. 3.9(c). Variation of the HH–LH band edge splitting at the well centre with indium content, for different values of $L_d$. The as-grown well width is $L_z = 10$ nm.
higher indium content, reflecting the higher strain present in the latter case. The decrease in the HH-LH band edge splitting with interdiffusion contributes to the decrease in the difference between the C1-HH1 and C1-LH1 transition energies that results with increasing L_d, shown in Fig. 3.7(b).

The variation of the HH-LH band edge splitting with well width, for three different stages of interdiffusion, is shown in Fig. 3.9(b). The splitting is greatest in the as-grown stage, and since the strain in the as-grown QW is independent of the well width (for wells within the critical thickness regime), the splitting is constant. After disordering, the indium content, and thus the strain, in the well depends on the as-grown well width, the larger the as-grown well width the higher the value of the indium content within the well for the same L_d, so that the HH-LH band edge splitting is larger for larger well widths. For a constant L_d/L_z ratio the variation in the HH-LH band edge splitting with L_d is independent of the as-grown well width, while it increases with increasing indium content. Fig. 3.9(c) shows the variation of the HH-LH band edge splitting with indium content, for three different values of L_d, for an as-grown well width of L_z = 10 nm. It can be seen that the higher the indium content of the as-grown QW, the larger is the variation in the band edge splitting with interdiffusion.

The above results are of interest since the HH-LH band edge splitting strongly influences the optical properties because of the polarisation dependence of the selection rules applying to optical transitions. The transition from the HH subband to the lowest conduction subband is allowed only for light polarisation parallel to the QW layer plane, the TE mode, while the corresponding LH transition is allowed for both the parallel polarisation and the polarisation in the z-direction, the TM mode.
3.4.2. Subband Structure

The effect of the coupling of the HH and LH subbands for the as-grown, and disordered ($L_d = 4 \text{ nm}$, and $L_d = 8 \text{ nm}$) QWs, is shown in Fig. 3.10, where the zero of energy is taken at the bottom of the HH confinement profile. The HH1 subband is not altered significantly with the inclusion of valence-band coupling since this subband is furthest removed from the LH1 subband. As already noted, in a compressively strained QW structure the uniaxial strain splits the HH and LH subbands and thus the mixing effect for the ground state hole subbands is reduced. Hence one would expect only a small change in the effective HH mass in the plane of the QW layer. The nonparabolicity is more pronounced in the case of LH1 subband so that a larger change in effective mass is expected. In the disordered QW more subbands arise and the subbands are closer together, but because of the compressive biaxial strain in InGaAs/GaAs QWs the LH1 band edge position is always furthest removed from the Cl subband. Thus the HH1 subband still exhibits low nonparabolic and band mixing effects as compared with the LH1 subband for $L_d < 8 \text{ nm}$.

The valence subband mixing and nonparabolicity effects in disordered, strained InGaAs/GaAs QWs are much less pronounced than in lattice-matched AlGaAs/GaAs QWs, because of the strain-induced HH-LH band edge splitting, as can be inferred by comparing HH1-LH1 band edge separation for the two material systems. The HH1-LH1 band edge separation for the as-grown $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$ single QW with $L_z = 10 \text{ nm}$ is $79 \text{ meV}$, and decreases with interdiffusion to $49 \text{ meV}$ when $L_d = 4 \text{ nm}$. The corresponding HH1-LH1 band edge separation in an $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}$ single QW with $L_z = 10 \text{ nm}$ are only $14 \text{ meV}$ and $7 \text{ meV}$, respectively. It has been shown that the reduced subband nonparabolicity results in a reduced valence-band density of states.
Fig. 3.10(a). Valence subband structure of a 10 nm $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$ single QW for $L_d = 0$. The zero of energy is taken as the bottom of the HH confinement profile.
Fig. 3.10(b). Valence subband structure of a 10 nm InGaAs/GaAs single QW for $L_d = 4$ nm. The zero of energy is taken as the bottom of the HH confinement profile.
Fig. 3.10(c). Valence subband dispersion of a 10 nm In$_{0.20}$Ga$_{0.80}$As/GaAs single QW for $L_d = 8$ nm. The zero of energy is taken at the bottom of the HH confinement profile. Counting up in the positive direction from this reference, the valence subbands are HH1, HH2, HH3, HH4, HH5, and LH1, respectively.
in compressively strained QW structures,\textsuperscript{3,58,59} and is attributed as one of the main factors for improved modulation bandwidth in strained QW lasers.\textsuperscript{3,58}

3.5. Summary

The effects of interdiffusion on the strain and confinement profiles in disordered InGaAs/GaAs single QWs have been studied, assuming an error function compositional distribution after interdiffusion. The compressive strain modifies the depths of the carrier confinement profiles so that, starting with a conduction-to-valence band offset ratio of 70:30, the presence of strain results, for the x = 0.2 structure, in a conduction-to-heavy hole effective offset ratio of 55:45 and a conduction-to-light hole effective offset ratio of 87:13. Disordering gives rise to graded strain profiles, which contribute to the modification of the carrier confinement profiles. As interdiffusion proceeds the depth of the confinement profiles (with a maximum at the QW centre) diminishes while the number of subband states increases. The changes in the confinement profiles are analyzed in terms of the cross-over point, defined as the potential of the graded confinement profile where the latter meets the as-grown confinement profile. Numerical results are presented for the subband energy levels, interband transitions energy and the square of the envelope integral, \(|<\chi_{cp}|\chi_{vq}>|^2\), for various stages of interdiffusion. The disordering process leads to an increase in the ground state C-HH transition energy, and reduces the HH-LH band edge splitting in strained InGaAs/GaAs QW structures. The enhancement of the off-diagonal \(|<\chi_{cp}|\chi_{vq}>|^2\) in the disordered QW indicates that the optical transition is sensitive to the profile shape. The results also show that the ground state transition energy variation with disordering is more sensitive to the indium content than to the well width of the as-grown QW, and that the variation in the HH-LH band edge splitting with disordering is larger for a higher indium content in the as-grown QW.
Consequently, it might be more favourable to start with an as-grown QW having as high a value of indium content as possible, keeping in mind the constraints of the critical thickness requirements for a coherently strained structure, in trying to tailor the carrier confinement profile of InGaAs/GaAs QWs by disordering.

The valence subband dispersion in InGaAs/GaAs single QWs is also determined using an effective Hamiltonian approach. The compressive strain in InGaAs/GaAs QWs results in significant HH-LH band edge splitting so that the heavy hole and light hole subband mixing effects are substantially reduced compared to AlGaAs/GaAs QWs. Although interdiffusion reduces the HH-LH band edge splitting, the ground state LH subband is always furthest from the ground state conduction subband so that the ground state HH subband still exhibits low nonparabolic and band mixing effects with interdiffusion for $L_d < 8$ nm.
3.6. References


OPTICAL ABSORPTION IN DISORDERED InGaAs/GaAs SINGLE QUANTUM WELLS

The change in the ground state transition energy that is observed with interdiffusion points to the possibility of tailoring the absorption edge of quantum well (QW) structures to desired wavelengths by means of QW disordering. This is of considerable interest in the design of photonic devices and an important requirement in the monolithic integration of these devices. In this chapter the effects of disordering on optical absorption in InGaAs/GaAs single QWs are investigated, taking into consideration interband transitions and excitonic contributions.

4.1. Introduction

Light is absorbed by the QW when a photon of sufficient energy excites an electron from the valence band into the conduction band, making an electron-hole pair. The lowest energy absorption occurs when the photon creates an electron-hole pair bound together in a state called an exciton. In an exciton, the electron and hole orbit around one another in a hydrogen-like state due to their electrostatic attraction. In QW structures the exciton is confined to a layer whose thickness is smaller than the excitonic Bohr diameter, so that the binding energy and oscillator strength of the exciton increase. Excitonic effects produce large absorption peaks just below the interband transition energy, which become stable even at room temperature, and which sharpen the absorption edge. Each interband transition exhibits an exciton peak at its onset and a correlation
enhanced continuum above.\(^4\)\(^6\) Well-resolved room temperature excitons first observed in AlGaAs/GaAs QW structures,\(^4\)\(^4\) have also been reported in several III-V material QW structures, including InGaAs/GaAs,\(^4\)\(^7\) and In\(_{0.53}\)Ga\(_{0.47}\)As/InP.\(^4\)\(^8\)

The strong excitonic absorption readily saturates at low powers compatible with laser diode sources.\(^4\)\(^4\) This room temperature nonlinearity has been exploited in optical switching devices.\(^4\)\(^9\) Another important property of the well resolved excitons at room temperature is the quantum-confined Stark effect (QCSE). When an electric field is applied perpendicular to the QW layer, the exciton peaks remain resolved up to very high fields and show significant shifts in absorption edge.\(^4\)\(^10\) The QCSE exhibited in QW structures has been applied in optical modulators\(^4\)\(^11\) and in self-electro-optic devices.\(^4\)\(^12\)

QW disordering also leads to significant shifts in the absorption edge of QW structures, as well as in the spectral peaks of QW lasers. Selective IID of a single QW laser structure has been used to shift the absorption edge to shorter wavelengths, obtaining a passive waveguide in the disordered section,\(^4\)\(^13\) thus integrating an active laser with a passive waveguide. IFVD has been employed to selectively shift the emission spectrum of a QW laser diode to higher energies.\(^4\)\(^14\)

### 4.2. Interband Optical Absorption

When an interband transition occurs in a QW the electron-hole pair form a dipole moment rotating in a plane perpendicular to the wave vector \(k\). Since the wave vector in the z-direction, the confinement axis, is now discrete, corresponding to the quantization of the energy levels, \(k\) itself takes discrete values and the dipole moment can rotate only in certain orbits, giving rise to polarisation dependence. For light propagating parallel to the QW layer, the electric field of the light parallel to the plane of the QW layer, the TE polarisation, interacts with the component of the dipole moment along the transverse
direction, and the electric field of the light perpendicular to the QW layer, the TM polarisation, interacts with the dipole moment component along the z-direction. At $k_{\parallel} = 0$ the heavy hole (HH) transition can only occur with TE polarised light, while the light hole (LH) transition occurs both for TE and TM polarisations.\textsuperscript{4,15} For light propagating perpendicular to the QW layer there is only one possible polarisation, the electric field of the light parallel to the QW layer plane, and the probability for HH transitions is three times larger than for LH transitions.\textsuperscript{4,16}

The interband transition probability for particles confined in a QW is the product of the square of the interband dipole matrix element, the electron-hole envelope function overlap integral, and the joint density of states.\textsuperscript{4,6} In the absence of excitonic effects the absorption coefficient should consist of a series of steps corresponding to the various allowed transitions, reflecting the 2D density of states. As already noted, the strength of an interband transition is reflected in the value of the overlap integral, while the observed transitions in finite QWs can be interpreted in terms of a relaxed selection rule, $p + q$ = even,\textsuperscript{4,17} where $p$, $q$ denote the conduction and valence subbands, respectively.

### 4.2.1. Absorption Coefficient and Dielectric Function

Optical properties can be described in terms of the complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The absorption coefficient $\alpha(\omega)$ is related to the imaginary part of the dielectric function by:\textsuperscript{4,18}

$$\alpha(\omega) = \frac{\omega}{n_r c_0} \varepsilon_2(\omega)$$

(1)

where $n_r$ is the refractive index, and $c_0$ is the speed of light in vacuum.

The contributions of direct interband transitions to $\varepsilon_2(\omega)$ for an undoped structure, using the dipole approximation,\textsuperscript{4,18} may be written as:\textsuperscript{4,19}
\( \varepsilon_2(\omega) = \frac{2}{\varepsilon_0 V} \sum_{p,q} \sum_{k_{||}} |<\chi_{cp}|\chi_{vq}>|^2 |\hat{\varepsilon}.M_{pq}|^2 G(E_{pq} - \hbar \omega) \delta [E_p(k) - E_q(k) - \hbar \omega] \) (2)

where \( \varepsilon_0 \) is the free space permittivity, \( V \) is the volume of the QW and the factor 2 results from spin considerations, \( k_{||} \) is the wave vector in the transverse plane (parallel to the well-barrier interface), \( |<\chi_{cp}|\chi_{vq}>|^2 \) is the overlap integral between the \( p \)th conduction subband and the \( q \)th valence subband due to the confinement effects of the envelope functions, \( \hat{\varepsilon} \) is a unit vector in the direction of the optical field, \( M_{pq} \) is the transition dipole matrix element between the \( p \)th conduction subband and the \( q \)th valence subband due to the effect of the periodic parts of the Bloch wave function, \( \delta \) is a Lorentzian function which represents the broadening effect due to interband relaxation by carrier-carrier scattering, \( \hbar \omega \) is the interband transition energy with a parabolic dispersion in the transverse direction for both conduction and valence subbands, \( \delta \) denotes the Dirac delta function, and \( \hbar \omega \) is the photon energy. Since the structure is assumed undoped, the conduction band is empty and the valence band is completely filled. The terms in eq. (2) are given by:

\[ <\chi_{cp}|\chi_{vq}> = \int \chi_{cp}^*(z) \chi_{vq}(z) dz \] (3)

\[ |\hat{\varepsilon}.M_{pq}|^2 = \frac{e^2 \hbar^2}{6m^*_c E_{pq}^2} M_0 \Theta(E) \] (4)

where

\[ E_{pq} = E_{cp} + E_{vq} + \tilde{E}_g + \frac{\hbar^2 k_{||}^2}{2\mu_{||CV}} \] (5)

\[ \frac{1}{\mu_{||CV}} = \frac{1}{m^*_c} + \frac{1}{m^*_{||V}} \] (6)
\[ M_\sigma = \frac{E_g (E_g + \Delta_g)}{E_g + \frac{2\Delta_o}{3}} \tag{7} \]

\[ \Phi\left( E_{pq} - \hbar\omega \right) = \frac{1}{\pi} \frac{\Gamma_b}{(E_{pq} - \hbar\omega)^2 + \Gamma_b^2} \tag{8} \]

e is the electronic charge, \( \Phi(E_f) \) is the polarisation factor describing the polarisation dependence, \( E_g \) is the unstrained bandgap of the interdiffused well at the well centre \( z = 0 \), \( \Delta_o \) is the spin-orbit splitting after interdiffusion at \( z = 0 \), \( \mu_{||CV} \) is the electron-hole reduced effective mass, \( \Gamma_b \) is the half width half maximum of the Lorentzian broadening, and \( z_b = 500 \) nm is taken as the limit of integration.

For incident light propagating parallel to the plane of the QW layer, the energy dependence of the polarisation factor \( \Phi(E_f) \) is defined by the following equations:\textsuperscript{4,22-4,23}

\[ \Phi^{TE} = \frac{3}{4} \left( 1 + E_R \right) \quad HH \]

\[ \Phi^{TM} = \frac{5}{4} \left( 1 - \frac{3}{5} E_R \right) \quad LH \tag{9} \]

\[ \Phi^{TM} = \frac{3}{2} \left( 1 - E_R \right) \quad HH \]

\[ \Phi^{TM} = \frac{1}{2} \left( 1 + 3E_R \right) \quad LH \tag{10} \]

where

\[ E_R = \frac{E_{cp} + E_{vq}}{E_{cp} + E_{vq} + E_i} \tag{11} \]

and \( E_t \) is the transverse energy, which, assuming a parabolic energy dispersion for both conduction and valence subbands, is given by:
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\[ E_1 = \frac{\gamma^2 k^2}{2\mu_1^*} \]  

(12)

Substituting eq. (3) to eq. (8) in eq. (2) gives

\[ \varepsilon_2(\omega) = \frac{e^2 \hbar^2}{3m^*_c e^*_o} \sum_{p,q} \langle \chi_{cp}\chi_{c q} \rangle \left| \frac{1}{2} \sum_{k_n} \frac{1}{E_{pq}^2} \mathfrak{g}(E_{pq} - \gamma \omega) \right| \]  

(13)

where the \( \delta \) has been omitted for simplicity. Assuming isotropic material, the summation over \( k_{||} \) can be converted into an integral over the transverse energy \( E_x \) as follows:

\[ \frac{1}{V} \sum_{k_n} \frac{\Theta(E_x) \mathfrak{g}(E_x)}{E_{pq}^2} = \frac{\mu_1^*}{2\pi \hbar^2 L_z} \int \frac{\Theta(E_x) \mathfrak{g}(E_{pq} - \gamma \omega)}{E_{pq}^2} \, dE_x \]  

(14)

where \( L_z \) is the QW width. \( \varepsilon_2(\omega) \) can now be expressed as:

\[ \varepsilon_2(\omega) = \frac{e^2 \Gamma_{p q} \mu_1^*}{6\pi^2 e^*_o L_z m^*_c} \sum_{p,q} \langle \chi_{cp}\chi_{c q} \rangle^2 I_{pq}(\gamma \omega) \]  

(15)

where

\[ I_{pq}(\gamma \omega) = \int \frac{\Theta(E_x)}{(E_{pq} + E_x)^2 [ (E_{pq} - \gamma \omega)^2 + \Gamma]^2} \, dE_x \]  

(16)

The summation in eq. (15) is over all the bound states, taking into consideration both HH-to-conduction and LH-to-conduction interband transitions.

4.2.2. Polarisation Dependent Interband Absorption Coefficient

The absorption coefficient spectra of disordered InGaAs/GaAs single QWs for incident light propagating parallel to the QW layer plane are calculated here for both TE and TM polarisation over a limited energy range above the bandgap in the T-valley,
where the quantization effects become evident. In order to demonstrate the effect of disordering on the absorption coefficient, calculations are carried out for an undoped In$_{0.5}$Ga$_{0.5}$As/GaAs single QW for $L_z = 10$ nm, and for various values of the diffusion length $L_d$ that characterises the disordering process. An error function compositional profile is assumed after interdiffusion. The material parameters used in the numerical calculations are as listed in Table 3.1, and in Table 4.1 below. A value of $\Gamma_b = 10$ meV was considered to be relevant to room temperature absorption spectra.$^{4.24,4.25}$

### Table 4.1.

*Material parameters used in calculations. (See also Table 3.1)*

<table>
<thead>
<tr>
<th></th>
<th>In$<em>x$Ga$</em>{1-x}$As</th>
<th>Units</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_r$</td>
<td>$12.85 - 2.30x$</td>
<td>$\varepsilon_0$</td>
<td>4.26, 4.27</td>
</tr>
<tr>
<td>$n_r$</td>
<td>$3.666 + 0.048x$</td>
<td>-</td>
<td>4.28</td>
</tr>
</tbody>
</table>

#### 4.2.2.1. Absorption Coefficient with Parabolic Band

The detailed results on the quantized energy levels, interband transitions energy, and electron-hole overlap integrals calculated within the parabolic band approximation in the last chapter are used to evaluate the polarisation dependent absorption coefficient. The interband absorption coefficient of the disordered InGaAs/GaAs QW as a function of wavelength for various values of $L_d$, for the TE and TM polarisations, are shown in Fig. 4.1. The absorption coefficient spectrum is a function of the number and strength of the allowed transitions, and of the individual contributions of the HH and LH transitions to the two polarisations, giving rise to the structure seen around the absorption
edge. This is particularly evident in the TE absorption spectra, shown in Fig. 4.1(a). The TM absorption coefficient spectra contain less structure, since the contributions of the HH transitions to this polarisation are much less, see Fig. 4.1(b), and only one confined LH subband is supported by the structure due to the presence of compressive strain. For the as-grown single QW the TE absorption edge is about 50 nm above the TM absorption edge, reflecting the large energy difference between the C1-HH1 and C1-LH1 transitions in the strained QW structure, which results from the HH-LH band edge splitting due to the uniaxial component of strain. Both TE and TM spectral absorption coefficient curves exhibit a smoother structure than corresponding ones for the AlGaAs/GaAs system, since the compressive strain in InGaAs/GaAs results in fewer confined subbands being supported.

In the initial stages of interdiffusion ($L_d = 1$ nm) the spectral absorption coefficient is very similar to that of the as-grown single QW structure since the dominant transitions hardly change. As the interdiffusion proceeds the absorption edge wavelength for both the TE and TM polarisations is blue shifted ($\Delta \lambda \approx 50$ nm for $\Delta L_d = 4$ nm for the TE case) and the spectral absorption coefficient has more structure. This is shown by the case of $L_d = 0.4L_c$ in Fig. 4.1(a) and reflects the fact that the nonlinear well potential profile now supports more confined states. However, at a larger value of $L_d$, ($L_d = 8$ nm), although still more confined subbands are supported, they are now more closely packed, resulting in a smoother profile while the peak absorption is also increased. For the case shown in Fig. 4.1(a) the absorption edge is shifted by $\approx 80$ nm while the peak absorption coefficient almost doubles as $L_d$ changes from $L_d = 0$ to $L_d = 8$ nm. In InGaAs/GaAs the shift in absorption edge results from the combined effects of compressive strain and disordering and occurs at a wavelength range which is higher than that achievable in the AlGaAs/GaAs system. Disordering in a strained...
Fig. 4.1(a). Spectral absorption coefficient curves for a 10 nm wide single 
In$_{0.2}$Ga$_{0.8}$As/GaAs disordered QW for TE polarisation for a range of diffusion 
lengths: $L_d = 0$ nm (solid line), $L_d = 1$ nm (dashed line), $L_d = 4$ nm (dotted-dashed line), 
$L_d = 8$ nm (dotted line).
Fig. 4.1(b). Spectral absorption coefficient curves for a 10 nm wide single
In$_{x2}$Ga$_{x3}$As/GaAs disordered QW for TM polarisation for a range of diffusion
lengths: $L_d = 0$ nm (solid line), $L_d = 1$ nm (dashed line), $L_d = 4$ nm (dotted-dashed line),
$L_d = 8$ nm (dotted line).
QW structure not only changes the bulk bandgap, but also alters the strain in the structure so that the strained bandgap of the disordered QW, and hence the absorption edge, is determined by disordering and strain, as well as carrier confinement effects.

It can be seen from Fig. 4.1 that the large wavelength separation (≈ 50 nm) between the TE and TM polarisation absorption edges for the as-grown QW decreases with interdiffusion, reflecting the reduced HH-LH band edge splitting. The results of Fig. 4.1 also suggest that it may be possible to achieve the same absorption edge for TM and TE polarisations at a given wavelength by suitable choice of L_d. This change in polarisation dependency with disordering in strained QW structures is of importance, in particular in polarisation sensitive applications.

Calculations were also carried out for different as-grown well widths, with L_d fixed at 0.4 L_z, and the results are presented in Fig. 4.2. Values of L_z = 5, 8, and 10 nm were used, so that the well widths do not exceed the relevant critical thickness. It is found that the absorption edge wavelengths for both TE and TM polarisation are red shifted towards longer wavelengths for increasing well widths, since as L_z increases the transition energies decrease. From Fig. 4.2(a) it can be seen that the absorption edge for the TE polarisation is shifted only by ≈ 15 nm as the well width doubles from 5 to 10 nm. The absorption spectra in Fig. 4.1 and Fig. 4.2 indicate that disordering can provide a wider range of wavelengths over which the absorption edge can be tailored than that possible by varying as-grown QW widths. The strain in a QW layer is independent of the QW thickness for a pseudomorphic structure so that in varying the QW width, the shift in the absorption edge is a function of the confinement effects only. For a constant L_d/L_z ratio the HH-LH band edge splitting is independent of the as-grown well width, as shown in chapter 3, and thus for the absorption spectra of Fig. 4.2, the shift in the absorption edge is again determined only by the carrier confinement effects.
Fig. 4.2(a). Spectral absorption coefficient curves for TE polarisation for a disordered \( \text{In}_{0.2}\text{Ga}_{0.8}\text{As/GaAs single QW, with } L_d = 0.4\ L_z\) for different as-grown QW widths: \( L_z = 10 \text{ nm (solid line)}, L_z = 8 \text{ nm (dotted-dashed line)}, L_z = 5 \text{ nm (dashed line)}.\)
Fig. 4.2(b). Spectral absorption coefficient curves for TM polarisation for a disordered InGaAs/GaAs single QW, with $L_d = 0.4 L_z$, for different as-grown QW widths: $L_z = 10$ nm (solid line), $L_z = 8$ nm (dotted-dashed line), $L_z = 5$ nm (dashed line).
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The results presented here show that the shape and position of the absorption edge are more sensitive to variations in well shape caused by the interdiffusion process than to the QW thickness, while the peak absorption is influenced by both the shape and thickness of the well. This shift in absorption edge in InGaAs/GaAs QWs results from the effects of disordering and compressive strain, and is moderated by the presence of strain in the QW structure. Thus strained QW structures can offer a higher sensitivity in varying the absorption edge, so that disordering can be an attractive proposition in tailoring the absorption edge of strained QW structures to desired wavelengths. These results can be useful in the monolithic integration of photonic devices. As an example, it should be possible, by careful use of selective disordering, to fabricate on a single substrate several lasers operating at different wavelengths. These can be included on a wafer with low loss waveguides in which the QW absorption is shifted to even shorter wavelengths. It should be noted that the above analysis, which excludes exciton effects, can be of interest in laser applications since the subband-to-subband optical gain can be calculated in a similar formulation.\textsuperscript{431}

4.2.2.2. Absorption Coefficient with Valence Subband Mixing

The interband absorption coefficient has also been obtained taking into account valence subband mixing. Using the dipole approximation,\textsuperscript{4,18} the absorption coefficient for an undoped QW structure can again be determined through the imaginary part of the dielectric function, and is given by:\textsuperscript{4,18}

\[
\alpha(\omega) = \frac{4\pi e^2}{\varepsilon_0 c^3 \hbar \omega m^*} \sum_{\nu \lambda} \left| \delta M_{\nu\lambda}(k_z) \right|^2 \delta [E_p(k_{||}) - E_q(k_{||}) - \hbar \omega] \frac{d^2k_{||}}{4\pi^2} \tag{17}
\]
where $e$ is the electronic charge, $\varepsilon_0$ is the free space permittivity, $n_r$ is the refractive index, $c_0$ is the speed of light in vacuo, $\hat{e}$ is a unit vector in the direction of polarisation of the optical field, and $M_{pq}(k_{||})$ is the momentum matrix element between the $p$th conduction subband and the $q$th valence subband. In evaluating the expression the $\delta$ function is replaced by a Lorentzian of half width half maximum $\Gamma_b$, which represents a broadening factor due to interband relaxation by carrier-carrier scattering.

The interband absorption coefficient of the disordered QW for various values of $L_d$ for TE and TM polarisation was determined using eq. (17) and the results are shown in Fig. 4.3. As in the case of the absorption coefficient with the parabolic band approximation, the structure observed here around the absorption edge reflects the number and strength of the allowed interband transitions and the polarisation dependence of the selection rules applying to optical transitions. Thus the TE spectra present more structure than the TM spectra, since in the latter case, the contributions of the HH transitions are much less and only one LH subband is supported due to the presence of the compressive strain.

As a result of interdiffusion the absorption edge wavelength for both TE and TM polarisations shifts to shorter wavelengths. For the TE polarisation, $\Delta \lambda \approx 50$ nm for $\Delta L_d = 4$ nm, and $\Delta \lambda \approx 80$ nm for $\Delta L_d = 8$ nm. The polarisation dependence of the absorption coefficient spectra can be also clearly observed, and again the large wavelength separation ($\approx 50$ nm) between the TE and TM polarisation absorption edges for the as-grown QW decreases with disordering.
Fig. 4.3(a). Absorption coefficient curves for TE polarisation, taking into account valence subband mixing, for a 10 nm wide single In$_{0.2}$Ga$_{0.8}$As/GaAs disordered QW for a range of diffusion lengths $L_d$. 
Fig. 4.3(b). Absorption coefficient curves for TM polarisation, taking into account valence subband mixing, for a 10 nm wide single In$_{0.2}$Ga$_{0.8}$As/GaAs disordered QW for a range of diffusion lengths $L_d$. 
4.3. Exciton Optical Absorption

The room temperature exciton binding energy and absorption coefficient spectrum of undoped, disordered InGaAs/GaAs single QWs are calculated here taking into consideration the 1S-like exciton, all the bound states, and the enhancement due to the 2D Sommerfeld factor for the continuum states. A parabolic band is assumed here, where band mixing is not considered, since as already noted, the compressive strain in InGaAs/GaAs QWs results in a large separation between the HH and LH subbands, greatly reducing band mixing effects.

4.3.1. Computational Considerations

The 1S bound exciton wave function is determined by a perturbation-variational method, and the variational parameter $\beta$ is obtained by minimizing the following:

$$
\int dz \int dz_v |\chi_{CI}(z_e)|^2 |\chi_{VI}(z_v)|^2 \left( \frac{1}{4} a_B + Z - \frac{1}{2} \pi Z [H_1(4\beta Z/a_B) - N_1(4\beta Z/a_B)] \right)
$$

where $z_e$ and $z_v$ represent the position of the electron and holes, $Z = |z_e - z_v|$, $\chi_{CI}$, $\chi_{VI}$ are the electron and hole envelope wave functions, $H_1$ and $N_1$ are the Struve and Neumann functions of order 1, respectively, and $a_B = 4\pi\varepsilon^2/(\mu^* c^3)$ is the exciton Bohr radius. The variational integral is obtained by employing a four point finite difference scheme per dimension.

The 1S exciton envelope function, $\chi_{1S}(\rho)$, and the exciton binding energy, $E_B$, are defined by:

$$
\chi_{1S}(\rho) = \frac{4\beta}{a_B/2\pi} \exp(-2\rho\beta/a_B)
$$

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\begin{equation}
E_b = -4\beta^2 R
\end{equation}

where $R = \mu^*_\parallel e^2/(32\pi^2\varepsilon^2\hbar^3)$ is the exciton Rydberg energy, and $\rho$ is the relative distance between the electron and hole in the QW along the transverse direction, which is parallel to the QW plane (i.e. the plane perpendicular to the growth direction $z$). The values for the HH and LH masses in the transverse direction, $m^*_\parallel_{\text{HH}}$ and $m^*_\parallel_{\text{LH}}$ respectively, are listed in Table 3.1.

The absorption coefficient of the disordered QW is calculated for the band edge $\Gamma$ region of the Brillouin zone, and includes the 1S exciton, and all the bound states, including the 2D enhancement Sommerfeld factor. The bound state absorption coefficient, $\alpha_{\text{bs}}(\omega)$, is given by:

\[ \alpha_{\text{bs}}(\omega) = \frac{e^2\mu^*_\parallel(\omega)}{6e_0C_R n_r m^*_e E_c^2 L_z} \tilde{M}_o \sum_{pq} |\langle \chi_{cp}|\chi_{pq} \rangle|^2 I_{pq}(h\omega) \]

where

\[ \tilde{M}_o = \frac{E_c(E_c + \Delta_o)}{E_c + 2\Delta_o} \]

\[ |\langle \chi_{cp}|\chi_{pq} \rangle| = \int_{x_0}^{x_s} \chi_{cp}(z)\chi_{pq}(z)dz \]

\[ I_{pq}(h\omega) = \int_0^\infty \Phi(E) S(E) \xi^2(E) dE \]

\[ S(E) = \frac{2}{1 + \exp(-2\pi \sqrt{R/E})} \]
\[
\mathcal{S}(E) = \frac{\Gamma_\parallel}{\pi((E_{CV} + E - \hbar\omega)^2 + \Gamma_\parallel^2)} \tag{26}
\]

S(E) is the Sommerfeld enhancement factor, \(\mathcal{S}(E)\) is the Lorentzian broadening factor, \(\mathcal{S}(E)\) is the polarisation factor, \(E_{CV} = \bar{E}_g + E_{Cl} + E_{Vd}\), \(\bar{E}_g\) is the interdiffusion induced bandgap at \(z = 0\), \(c_o\) is the velocity of light in free space, \(\varepsilon_o\) is the permittivity in free space, \(m^*_e\) is the effective electron mass, and the other standard physical constants have their usual values.

For light propagating perpendicular to the QW layer there is only one possible polarisation (the electric field of the light parallel to the plane of the QW layer) and the polarisation factor is given by \(\mathcal{P} = 3/2\ (HH), 1/2\ (LH)\). \(^4\) In the waveguide geometry, with light propagating parallel to the QW layer, the TE polarisation (the electric field of the light parallel to the plane of the QW layer), and the orthogonal polarisation (the electric field of the light perpendicular to the QW layer), called TM polarisation, occur. The polarisation factor now accounts for both the TE and TM polarisations, and is given by:

\[
\mathcal{P}^{TE} = \frac{3}{4} (1 + E_R) \quad HH \\
= \frac{5}{4} (1 - \frac{3}{5} E_R) \quad LH 
\tag{27}
\]

\[
\mathcal{P}^{TM} = \frac{3}{2} (1 - E_R) \quad HH \\
= \frac{1}{2} (1 + 3E_R) \quad LH 
\tag{28}
\]

where \(E_R = (E_{cp} + E_{Wd})/(E_{cp} + E_{Vd} + E)\).

The exciton absorption coefficient, \(\alpha_{exc}(\omega)\), is given by:
\[ \alpha_{1s}(\omega) = \frac{A \omega}{c \mu_r} \left| \chi_{1s}(\omega) \right|^2 \frac{\Gamma_b}{\pi (E_{\text{exc}} - \gamma_\omega)^2 + \Gamma_b^2} \]  

(29)

\[ A = \frac{e^2 h^2}{3 e_0 m^* E_{\text{C}} L_z} \langle \chi_{C} | \chi_{V} \rangle \langle \chi_{V} | \chi_{C} \rangle \phi^2 \]  

(30)

where \( E_{\text{exc}} = E_{\text{C}} + E_{\text{v1}} + E_{\text{b}} + E_{\text{p}} \) and \( \Gamma_b \) is the exciton linewidth (half width half maximum) broadening factor. For the 1S exciton only \( \rho = 0 \) is allowed and hence \( \phi^\text{TH} = 3/2 \) (HH), \( 1/2 \) (LH) and \( \phi^\text{TM} = 0 \) (HH), 2 (LH).

### 4.3.2. Results and Discussion

The In\(_x\)Ga\(_{1-x}\)As/GaAs single QW structure considered here has an as-grown well width \( L_x = 10 \) nm, \( x = 0.20 \). The same material parameters used in the computation of the interband optical absorption coefficient spectra are used in the numerical calculations here.

The exciton binding energy for both heavy hole and light hole is shown in Fig. 4.4(a). The solid curves give the exciton binding energy using strain-independent carrier effective masses along the quantization axis, as obtained from a linear interpolation between the values for the binary compounds. The dashed curves give the exciton binding energy taking into consideration strain-dependent electron and LH effective mass along the quantization axis, calculated using a model developed in Ref. 4.39. The HH effective mass remains within the parabolic band approximation along the quantization axis.\(^{4.39} \) It can be seen that taking strain-dependent masses increases the exciton binding energy for both HH and LH but only by a small amount, about 0.3 meV. This difference is reduced with interdiffusion since, as interdiffusion
proceeds, the In content in the QW decreases, thereby reducing the strain in the QW. Since the change in the exciton binding energy when considering strain-dependent masses is small, the parabolic band approximation is used in the rest of the calculations.

It can be seen from Fig. 4.4(a) that the heavy hole exciton binding energy increases during the initial stages of interdiffusion ($L_d \leq 1.8$ nm) and then decreases as interdiffusion proceeds further. The light hole exciton binding energy, on the other hand, decreases monotonically as $L_d$ increases. These variations can be explained in terms of the variations of the $\ell = 1$ subband states $E_{ci}$, $E_{HH}$, $E_{LH}$ with $L_d$, shown in Fig. 4.4(b). The electron and HH ground state experience an effectively narrower well than the as-grown well width during the initial stages of interdiffusion so that both $E_{ci}$ and $E_{HH}$ (measured from the bottom of the respective confinement profile) increase initially, as shown in Fig. 4.4(b). As interdiffusion proceeds further the ground state electron and HH experience an effectively wider well than the as-grown well width so that now both $E_{ci}$ and $E_{HH}$ decrease. In the case of the LH, however, the confinement profile differs from the HH confinement profile because of the strain-induced HH-LH splitting. As a result the well width experienced by the LH ground state is effectively unchanged from the as-grown well width, in the early stages of interdiffusion, so that $E_{LH}$ does not change. As interdiffusion proceeds further, the well experienced by the LH ground state becomes effectively wider than the as-grown well and $E_{LH}$ now decreases. The results shown in Fig. 4.4(a) thus indicate the sensitivity of the exciton binding energy to the carrier confinement profile.

The LH exciton binding energy is less than the HH exciton binding energy. This is in contrast to lattice-matched AlGaAs/GaAs QW structures, where the LH exciton binding energy is greater than the HH exciton binding energy, and is a direct result of the presence of compressive strain in the InGaAs/GaAs QW structure. The exciton
Fig. 4.4. (a) The heavy hole (HH) and light hole (LH) exciton binding energy variation with $L_d$ for a single $\text{In}_{0.2}\text{Ga}_{0.8}\text{As/GaAs QW}$ with $L_z = 10$ nm. The solid curves refer to calculations with strain-independent carrier effective masses, dashed curves refer to results with strain-dependent effective masses. (b) The electron (C1), heavy hole (HH1), and light hole (LH1) ground state energy level variation with $L_d$. 

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binding energy is a function of the in-plane reduced mass, \( \mu_{\parallel,cv}^* \) and, through \( \beta \), of the envelope wave function. In AlGaAs/GaAs QWs the HH and LH valence bands are degenerate at the \( \Gamma \) valley and thus the ground state HH and LH wave functions are equally confined. (There is only a 5% difference in the values of the HH and LH \( \beta \)'s in AlGaAs/GaAs.) Thus the exciton binding energy is mainly a function of the in-plane reduced mass \( \mu_{\parallel,cv}^* \) in AlGaAs/GaAs. Since \( \mu_{\parallel,cv}^* = \frac{m_{\parallel}^*}{c(1 + m_{\parallel}^* c / m_{\parallel}^* v)} \), \( \mu_{\parallel,ch}^* < \mu_{\parallel,cl}^* \) so that the HH exciton binding energy is smaller than the LH binding energy. In InGaAs/GaAs \( \mu_{\parallel,ch}^* \) is again less than \( \mu_{\parallel,cl}^* \), but the strain-induced HH-LH confinement profile splitting at \( \Gamma \) causes the depth of the LH confinement profile to be shallower than the depth of the HH confinement profile by a factor of 5, for the case considered here. As a result the LH ground state wave function is much less confined than the HH ground state wave function, as shown in Fig. 4.5, so that \( \beta \) in the case of LH is now about 15% less than that of the HH. Consequently, the LH exciton binding energy is smaller than the HH exciton binding energy in InGaAs/GaAs.

The ground state heavy hole and light hole excitonic transition energy variation with \( L_d \) are shown in Fig. 4.6(a). The heavy hole transition is the QW bandgap energy and this is a result of the compressive nature of the strain in the QW. As \( L_d \) increases the ground state heavy hole exciton transition energy also increases, as evidenced in experimental results. The QW bandgap energy shift due to disordering, is shown in Fig. 4.6(b), for both heavy hole and light hole excitons. It can be seen that this shift is much larger for the heavy hole than for the light hole. This is a result of the strain-induced HH-LH band edge splitting. A change in \( L_d \) from 0 to 6 nm corresponds to a change in heavy hole transition energy of about 100 meV, which represents a shift to shorter wavelengths of about 80 nm, whereas the corresponding light hole transition
Fig. 4.5. Normalized wave function squared for ground state HH and LH.
Fig. 4.6. (a) HH and LH ground state exciton transition energy variation with $L_d$.

(b) HH and LH ground state exciton transition energy shift with $L_d$. 
energy changes by about 55 meV, representing a shift to shorter wavelengths of about 45 nm. The results from the model, for the change in heavy hole excitonic transition energy with $L_d$, have been compared to photoluminescence data published recently.\textsuperscript{4,41} A calculated value of 47 meV results for the HH shift (with appropriate changes in parameter values to take account of the 77 K measurement temperature) for a single In$_x$Ga$_{1-x}$As/GaAs QW with $L_z = 10$ nm, $x = 0.24$, and $L_d = 2.5$ nm, which is in very good agreement with the published value of 50 meV.

The absorption coefficient, including the 1S exciton, is obtained from

$$\alpha(\omega) = \alpha_{bd,HH}(\omega) + \alpha_{bd,LH}(\omega) + \alpha_{1S,HH}(\omega) + \alpha_{1S,LH}(\omega)$$  \hspace{1cm} (31)$$

The absorption coefficient spectrum for light propagating perpendicular to the QW plane is shown in Fig. 4.7. The absorption spectrum exhibits two peaks superimposed on a stepwise curve. The stepwise absorption reflects the two dimensionality in the density of states due to quantum confinement, while the exciton resonance produces the absorption peaks and results in a sharper absorption edge. The dominant absorption peak, at 1.24 eV, is due to the $\ell = 1$ heavy hole exciton resonance. The effect of the $\ell = 1$ light hole exciton is less marked since the LH oscillator strength is much less than the HH oscillator strength, but can still be seen at 1.32 eV. In contrast with AlGaAs/GaAs QWs,\textsuperscript{4,37} the separation between the heavy hole and light hole exciton peaks is large and reflects the strain-induced HH-LH band edge splitting. The absorption spectrum for the as-grown QW ($L_d = 0$), shown in Fig. 4.7, compares well in trend with measured absorption spectra of InGaAs/GaAs square QWs at room temperature.\textsuperscript{4,24,43} Fig. 4.7 also shows the effect of disordered on the absorption spectrum. The heavy hole exciton peak shifts to higher energy with interdiffusion. This reflects the increase in bandgap energy which results in the disordered region due to the reduced In content and the consequent decrease in the strain. The effect of the light hole exciton at large $L_d$ is
Fig. 4.7. Absorption coefficient for different values of $L_d$, for incident light propagating perpendicular to the QW layer.
barely discernible since the C1-LH1 transition energy tends to merge with the C2-HH2 transition energy. The separation between the heavy hole and light hole exciton peaks is reduced, reflecting the reduced strain in the disordered QW structure.

For light propagating along the plane of the QW the absorption is polarisation sensitive. The absorption spectrum for the TE polarisation is shown in Fig. 4.8. Both the heavy hole exciton resonance, which dominates the TE absorption spectrum, and the light hole exciton peak can be seen. With increasing $L_d$ the heavy hole exciton related peak, which determines the absorption edge of the structure, shifts to shorter wavelengths. It can be seen from Fig. 4.8 that by careful control of the disordering process, the absorption edge can be tuned to a specific wavelength, while at the same time the exciton peaks remain fairly constant. The TM polarisation absorption spectrum is shown in Fig. 4.9. Only one LH confined subband is supported by the QW structure due to the compressive strain, and since only light holes contribute to TM polarisation absorption, a single absorption peak results. The absorption peak for the as-grown QW is about 60 nm below the dominant TE absorption peak, reflecting the large strain-induced separation between the C1-HH1 and C1-LH1 transitions. The TM absorption peak again shifts to shorter wavelengths with increasing $L_d$, but the corresponding shift in wavelength with $L_d$ is smaller than that which results for the TE case. The TE and TM absorption peaks move closer with disordering since the reduced strain in the QW after interdiffusion means a reduced HH-LH band edge splitting. Even so, a separation of about 35 nm still remains after interdiffusion for $L_d = 4$ nm. Thus, due to strain-induced HH-LH band edge splitting, the sensitivity of these strained QW structures to polarisation is greater than that in lattice-matched structures and is of importance for device design.

For the structure considered here, the TE absorption exciton peaks for $L_d = 0$ and, say, $L_d = 4$ nm, occur at 1.0 $\mu$m and 0.943 $\mu$m, respectively. This shift in absorption
Fig. 4.8. Absorption coefficient for different values of $L_d$ for TE polarisation, with incident light propagating parallel to the QW layer.
Fig. 4.9. Absorption coefficient for different values of $L_d$, for TM polarisation, with incident light propagating parallel to the QW layer.
exciton peaks with disordering can be of use in integrated optics. As an example, a

two-wavelength demultiplexing waveguide photodetector has been demonstrated in a

GaAs/AlAs multiple QW (MQW) structure, where the MQW absorbing layer was
divided into two sections with different absorption edges, by disordering a section of the

MQW structure. Different disordering process parameters, corresponding to different

values of $L_d$, will result in selective absorption edges so that in principle several

absorption sections with different absorption edges can be integrated in the same
demultiplexer. Sharp excitonic peaks are desirable in such an application and determine

the wavelength spacing of the channels. This requires a low value of the broadening

parameter $\Gamma_b$, and therefore demands structural high quality of the material, and of the

interface. This reduces the contributions to $\Gamma_b$ due to strain distribution (particularly in

strained QW structures), or interface roughness. In addition, use of single QWs, instead

of MQW structures, will also reduce the value of $\Gamma_b$, since no contributions will result

from variations in well width as would be observed in a MQW or superlattice.

Recently a two-wavelength demultiplexing photodetector, using IFVD disordering of a

single InGaAs/GaAs strained layer QW structure has been reported.

4.4. Summary

Calculated results of the absorption coefficient for direct interband optical

transitions have been carried out for both TE and TM polarisations, for disordered

InGaAs/GaAs single QWs, assuming an error function compositional profile after

interdiffusion. The shape and position of the absorption coefficient spectra are a function

of the confinement profile that results from the interdiffusion process, determined by the

combined effects of disordering and strain, and reflect the allowed interband transitions,

the value of the corresponding electron-hole overlap integral, and the individual HH and
LH contributions to the absorption coefficient for the two polarisations. Absorption coefficient spectra are presented for different interdiffusion stages and for different as-grown well widths, showing that the shift to shorter wavelengths that results in the absorption edge is affected more by disordering than by the QW thickness, while the peak absorption is influenced by both the shape and thickness of the well. Disordering can thus be an attractive proposition in tailoring the absorption edge.

The excitonic effects on the absorption coefficient spectra of disordered InGaAs/GaAs single QWs are also studied. The exciton binding energy variation with interdiffusion for both the HH and LH exciton are presented showing the sensitivity of the exciton binding energy to the carrier confinement profiles of the disordered QWs. The absorption coefficient spectra, for light propagating parallel to the QW layer and for normal incidence, are then determined within the parabolic band approximation, taking into consideration the 1S-like exciton, all the bound states, and the enhancement due to the 2D Sommerfeld factor for the continuum states. The absorption coefficient spectra exhibit well defined excitonic peaks which shift to shorter wavelengths with interdiffusion. The excitonic peaks in TE polarisation remain constant with interdiffusion and exhibit a larger wavelength shift than in TM polarisation. The absorption edge in disordered InGaAs/GaAs can be tailored to desired wavelengths around 1.0 μm. The results also show a large polarisation sensitivity which is a result of the compressive strain in the InGaAs layer. This polarisation sensitivity, reflected in a significant separation between the absorption edge for TE and TM polarisations for the as-grown QW, decreases with increasing interdiffusion. The above results can be applied to the design of photonic devices on a single substrate, such as multiple wavelength demultiplexers, and have implications for polarisation-sensitive applications.
4.5. References

Chapter 5

REFRACTIVE INDEX OF DISORDERED InGaAs/GaAs SINGLE QUANTUM WELLS

The refractive index is another important optical property which is significantly affected by the modifications in the subband structure that result in disordered, strained quantum wells (QWs). This change in refractive index caused by disordering can be exploited for the lateral confinement of photons, which is of particular importance for photonic devices such as waveguides and modulators. In this chapter the polarisation dependent refractive index of an InGaAs/GaAs single QW structure for as-grown and disordered sections is first determined, and the lateral refractive index step that results between as-grown and disordered regions is then obtained for wavelengths above 1 μm. The effects of disordering on the birefringence are also considered.

5.1. Introduction

A necessary prerequisite for the integration of semiconductor lasers with waveguides and modulators is the ability to strongly confine the laser output in both the lateral and vertical directions. This requires a positive refractive index step between the guiding section and the confining regions. Compositional and/or carrier concentration variations can be used to provide lateral as well as vertical confinement. Cladding layers with a higher bandgap energy provide vertical photon confinement, while selective area QW disordering can prove useful in obtaining a positive lateral refractive index step in QW structures, because of the change in the refractive index caused by disordering.
This change in refractive index is more pronounced near the fundamental absorption edge, but it remains significant at wavelengths above 1 μm, so that it is potentially useful at fibre optic communication wavelengths.

**5.2. Polarisation Dependent Refractive Index**

The first reported calculations of the polarisation dependent refractive index of disordered InGaAs/GaAs single QWs, where the light propagates in the plane of the QW layer, are presented here and discussed. The disordering process, which results in the interdiffusion of In and Ga atoms across the well-barrier interface,

\[ L_d = (Dt)^{1/2} \]

where \( D \) is the diffusion coefficient and \( t \) is the thermal processing time. The compositional profile of the disordered QW structure is described by an error function distribution.

**5.2.1. Refractive Index and Dielectric Function**

The refractive index, \( n_r \), is calculated using the complex dielectric function, by considering the contributions from the \( \Gamma, X, \) and \( L \) valleys of the Brillouin zone. The \( \Gamma \)-valley contribution is determined by a QW calculation using the Kane \( k\cdot p \) method for a four band model, while the \( X \) and \( L \) regions contributions are obtained using a bulk calculation, since the latter contributions to the band-edge of the QW structure affect only the magnitude of \( n_r \). The barrier is taken into account by introducing a 1:1 weighting between the well and barrier for the relevant calculations and material parameters.

The contributions of the \( X \) and \( L \) regions to the imaginary part of the dielectric function, \( \varepsilon_2^X(\omega) \) and \( \varepsilon_2^L(\omega) \), are negligible for the wavelength of interest, \( \lambda > 0.90 \) μm.
The contribution of the $\Gamma$-valley, $\varepsilon_2^\Gamma(\omega)$, is determined by considering all the bound states and 1S exciton contributions. A parabolic band structure is assumed and band-mixing is not considered, since the compressive strain in InGaAs/GaAs QWs results in a large separation between the heavy hole (HH) and light hole (LH) subbands, greatly reducing band-mixing effects.\(^5\) Details of the interdiffusion induced confinement profiles and the subband edge calculations,\(^6\) using spatially dependent effective masses and strain effects, are as presented in chapter 3, while the 1S exciton effect, calculated using a perturbative-variational approach, is described in chapter 4. $\varepsilon_2^\Gamma(\omega)$ is thus obtained from:

\[
\varepsilon_2^\Gamma(\omega) = \varepsilon_2^{bd}(\omega) + \varepsilon_2^{exc}(\omega)
\]

(1)

where $\varepsilon_2^{bd}(\omega)$ is the conduction-valence band bound state contribution, taking into consideration the 2D enhancement Sommerfeld factor, and obtained by summing over all the bound states for the conduction ($p$) and valence ($q$) bands, and $\varepsilon_2^{exc}(\omega)$ is the 1S exciton contribution derived by the density-matrix approach at the subband edge,\(^5\)\(^9\) and which are given by:

\[
\varepsilon_2^{bd}(\omega) = \frac{e^2\mu_{||}}{6\varepsilon_0 m_p^* E_{CV} L_z} \tilde{M}_o \sum_{p<q} |\langle \chi_{pq} | \chi_{pq} \rangle|^2 \int_0^\infty \left( \Phi(E) S(E) \mathcal{G}(E) - E - \hbar \omega \right) dE
\]

(2)

and

\[
\varepsilon_2^{exc}(\omega) = \frac{e^2 h^2 \Phi}{3\varepsilon_0 m_p^* E_{CV} L_z} \tilde{M}_o |\langle \chi_{pq} | \chi_{pq} \rangle|^2 |\chi_{1s}(p=0)|^2 \mathcal{G}(E - \hbar \omega)
\]

(3)

where $\Phi$ is the polarisation factor at the band edge, with $\Phi^{\\text{TH}} = 3/2$ (HH), $1/2$ (LH) and $\Phi^{\\text{TM}} = 0$ (HH), $2$ (LH); $S$ is the Sommerfeld enhancement factor,\(^5\)\(^10\) $\mathcal{G}$ is the Lorentzian broadening factor with a half width half maximum $\Gamma_b$; $\tilde{M}_o = \tilde{E}_g (\tilde{E}_g + \tilde{\Lambda}_0)/(\tilde{E}_g + 2\tilde{\Lambda}_0/3)$;
\( \tilde{E}_g \) is the interdiffusion induced bandgap at the QW centre; \( E_p, E_q, \) and \( E_{exc} \) are the electron subband energy, hole subband energy, and exciton transition energy, respectively; \( E_{CV} = \tilde{E}_g + E_{c1} + E_{V1}; \chi_e, \chi_h, \chi_{e+h} \) are the envelope wave functions for the electrons, the holes, and the exciton, respectively; \( \varepsilon_0 \) is the permittivity of free space; \( \mu^* || \) is the in-plane reduced mass; \( m_e^* \) is the electron effective mass along the quantization axis \( z; \) and \( L_z \) is the as-grown QW width centred at \( z = 0. \) The QW contribution, \( \varepsilon_1^{\Gamma, qw}(\omega), \) to the real part of the dielectric function, is determined using a Kramers-Kronig transformation of \( \varepsilon_2^{\Gamma}(\omega), \) taking into consideration the well-barrier weighting, and is given by:

\[
\varepsilon_1^{\Gamma, qw}(\omega) = 1 + \frac{2 \pi}{\omega} \int_0^\omega \frac{\omega' \varepsilon_2^{\Gamma}(\omega')}{\omega^2} d\omega'
\]

(4)

where \( P \) denotes the Cauchy principal value of the integral. This QW contribution and the \( \Gamma \)-valley continuum contribution, obtained using a bulk calculation,\(^5,^4\) are then weighted differently, according to the extent of interdiffusion, to obtain the final value of the \( \Gamma \)-valley contribution, \( \varepsilon_1^{\Gamma}(\omega), \) to the real part of the dielectric function. The \( X \) and \( L \) contributions to \( n_\gamma \) are calculated from the real part of the dielectric function \( \varepsilon_1^{X,L}(\omega) \) only, since \( \varepsilon_2^{X,L}(\omega) = 0 \) for the wavelength range of interest. These bulk contributions are averaged continuously for the nonlinear profile within the well and the barrier before being weighted 1:1 between well and barrier. The real part of the dielectric function is then obtained from \( \varepsilon_1^{\gamma}(\omega) = \varepsilon_1^{\Gamma}(\omega) + \varepsilon_1^{X,L}(\omega). \) The real part of \( n_\gamma \) is determined by using the dielectric functions,\(^5,^11\) and is given by:

\[
n_\gamma = \frac{1}{2} \varepsilon_1^{\Gamma}(\omega) + \frac{1}{2} [\varepsilon_1^{\gamma}(\omega)]^2 + \varepsilon_2^{\gamma}(\omega)]^{\gamma^{1/2}}
\]

(5)
5.2.2. Results and Discussion

The room temperature refractive index \( n_r \) is calculated here for the wavelength range 0.87 \( \mu \text{m} \) to 2 \( \mu \text{m} \), for a pseudomorphic In\(_x\)Ga\(_{1-x}\)As single QW with thick (100 nm) GaAs barriers, where the InGaAs layer is under compressive strain and the GaAs barriers are unstrained. A conduction band offset ratio at \( \Gamma \)-point of 70:30\(^*\) is used in the QW calculations.

The refractive index spectra for TE polarisation in the wavelength range 0.88 \( \mu \text{m} \) to 1.68 \( \mu \text{m} \) are shown in Fig. 5.1. The as-grown single QW is defined by \( L_z = 10 \text{ nm} \), and \( x = 0.2 \). For \( \lambda > 1.0 \mu \text{m} \), the refractive index of the disordered QW decreases as \( L_d \) increases. During interdiffusion, the compositional profile, and the consequent strain modification, result in an increase of the ground state transition energy, with a consequent decrease in \( n_r \). For the structure considered here the In concentration at the well centre decreases by 5%, 32%, and 29%, respectively, and the ground state transition energy shifts by 28 meV, 44 meV, and 28 meV\(^*\), respectively, as \( L_d \) increases from 0 to 2 nm, 2 nm to 4 nm, and 4 nm to 6 nm, respectively. The decrease in \( n_r \) as \( L_d \) changes from 2 nm to 4 nm is thus more pronounced than the corresponding decrease as \( L_d \) varies from 0 to 2 nm, and from 4 nm to 6 nm. Note that although the decrease in In concentration at the well centre as \( L_d \) varies from 4 nm to 6 nm is about 6 times larger than that when \( L_d \) varies from 0 to 2 nm, the ground state transition energy increases by an equal amount for the two \( L_d \) ranges. This is due to the fact that as \( L_d \) increases above 4 nm, the electron ground state sees an effectively wider well than the as-grown well (see Fig. 3.3). The changing compositional profile with \( L_d \) is reflected also in the bulk contributions to \( n_r \) since they are averaged continuously over the error function profile within the well and the barrier. Towards the exciton edge, \( \lambda \approx 1.05 \mu \text{m} \), the \( n_r \) spectra rise to a peak. The fine structure
Fig. 5.1. The refractive index spectra for TE polarisation for various values of interdiffusion length $L_d$, for disordered In$_x$Ga$_{1-x}$As/GaAs single QWs. The as-grown QW details are $L_z = 10$ nm, $x = 0.2$. $L_d = 0$ (solid line), $L_d = 2$ nm (dot-dashed line), $L_d = 4$ nm (long dashed line), $L_d = 6$ nm (dotted line), $L_d = 10$ nm (short dashed line). The GaAs bulk refractive index is shown for reference.
at wavelengths immediately below the exciton edge, \( \lambda < 1.01 \mu m \), is due to the contribution from different bound state transitions in the QW. As \( L_d \) increases the peak at the band edge wavelength shifts to shorter wavelengths and as \( L_d \to \infty \), \( n_r \) approaches the value for bulk GaAs obtained from the bulk model.\(^5\)\(^4\) At even shorter wavelengths, calculations show that the \( n_r \) spectra decrease but eventually rise again at wavelengths below 0.5 \( \mu m \) where they reach the dispersion edges of the \( X \) and \( L \) valleys. The \( n_r \) spectra for the TM polarisation, shown in Fig. 5.2, are similar to those of the TE case except that they exhibit less structure near the exciton edge. This is due to the fact that the strain-induced HH-LH band edge splitting results in only one light hole subband being supported for all values of \( L_d \) considered here, in contrast to the HH case where more than a single subband is supported.\(^5\)\(^8\)

Calculations for a narrower as-grown well \( (L_z = 5 \text{ nm}, \ x = 0.2) \) show similar \( n_r \) wavelength spectra with increasing interdiffusion, with the exciton band edge shifting to shorter wavelengths \( (\lambda = 0.98 \mu m, \ at \ L_d = 0 \text{ nm}) \). The \( n_r \) spectra for TE polarisation, shown in Fig. 5.3(a), exhibit less structure just below the exciton edge because of the reduced density of states in the narrower well. The corresponding \( n_r \) spectra for a QW structure with an as-grown \( L_z = 5 \text{ nm}, \ x = 0.3, \) illustrated in Fig. 5.3(b), show that keeping the well width constant and increasing the In content shifts the exciton band edge to longer wavelengths \( (\lambda = 1.0 \mu m, \ at \ L_d = 0 \text{ nm}) \), since the depth of the confinement profiles is now larger, while interdiffusion again shifts the peak at the QW band edge wavelengths to shorter wavelengths. In comparison with the \( n_r \) spectra for the as-grown \( L_z = 10 \text{ nm} \) well, the refractive index for the \( L_z = 5 \text{ nm} \) QWs rises more sharply to its peak at the QW band edge wavelength. This is a result of the increased exciton binding energy in the narrower wells,\(^5\)\(^{13}\) resulting in enhanced excitonic resonance.
Fig. 5.2. The refractive index spectra for TM polarisation for various values of interdiffusion length $L_d$, for disordered In$_x$Ga$_{1-x}$As/GaAs single QWs. The as-grown QW details are $L_x = 10$ nm, $x = 0.2$. $L_d = 0$ (solid line), $L_d = 2$ nm (dot-dashed line), $L_d = 4$ nm (long dashed line), $L_d = 6$ nm (dotted line), $L_d = 10$ nm (short dashed line). The GaAs bulk refractive index is shown for reference.
Fig. 5.3. The refractive index spectra, for TE polarisation, for various values of interdiffusion length $L_d$, for disordered $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ single QWs, for (a) an as-grown $L_z = 5\text{ nm}$, $x = 0.2$, and (b) $L_z = 5\text{ nm}$, $x = 0.3$. $L_d = 0$ (solid line), $L_d = 1\text{ nm}$ (dot-dashed line), $L_d = 2\text{ nm}$ (long dashed line), $L_d = 3\text{ nm}$ (dotted line), $L_d = 5\text{ nm}$ (short dashed line). The GaAs bulk refractive index is shown for reference.
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5.3. Refractive Index Step

The refractive index step $\Delta n_t$ is here defined as the difference between the refractive index of an as-grown region and that of a disordered region, $\Delta n_t = n_t(L_d = 0) - n_t(L_d)$. The wavelength spectra for the refractive index step, shown in Fig. 5.4 for TE polarisation, are always positive for wavelengths $> 1 \mu m$, indicating that lateral photon confinement in the as-grown region is possible. The refractive index step is a function of the extent of interdiffusion, increasing as $L_d$ increases, and is positive also for $n_t(L_{d1}) - n_t(L_{d2})$, where $L_{d1} < L_{d2}$. The refractive index step in the InGaAs/GaAs structure considered here is less than the corresponding refractive index step for an Al$_{0.3}$Ga$_{0.7}$As/GaAs single QW with the same as-grown QW width. The carrier confinement profiles of the strained InGaAs/GaAs structure are considerably shallower than those in the AlGaAs/GaAs structure because the GaAs barrier band edge energy is smaller than the Al$_{0.3}$Ga$_{0.7}$As barrier band edge energy, and the strain in the InGaAs well increases the QW bandgap energy. As a result the ground state transition energy shift, and thus the decrease of $n_t$ with $L_d$, are larger in the Al$_{0.3}$Ga$_{0.7}$As/GaAs than in In$_{0.2}$Ga$_{0.8}$As/GaAs. The refractive index step is positive down to the as-grown QW exciton band edge while at shorter wavelengths, the sign of $\Delta n_t$ is more complicated so that its interpretation at these wavelengths is not straightforward. Similar results are obtained for the refractive index step spectra for TM polarisation, shown in Fig. 5.5. The values of $\Delta n_t$ obtained for both TE and TM polarisations for $L_d > 2 \mu m$, for wavelengths $> 1 \mu m$, are an order of magnitude larger than the refractive index step values typically obtained for free-carrier compensation techniques in optical waveguides, making QW disordering an attractive process for strong lateral photon confinement. A schematic diagram illustrating the potential use of disordering for the...
Fig. 5.4. Wavelength spectra for TE polarisation of the lateral refractive index step,
$\Delta n_t = n_t(L_d = 0) - n_t(L_d)$, for various values of interdiffusion length $L_d$. The as-grown
In$_x$Ga$_{1-x}$As/GaAs single QW details are $L_z = 10$ nm, $x = 0.2$. 

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Fig. 5.5. Wavelength spectra for TM polarisation of the lateral refractive index step, \( \Delta n_r = n_r(L_d = 0) - n_r(L_d) \), for various values of interdiffusion length \( L_d \). The as-grown \( \text{In}_{x}\text{Ga}_{1-x}\text{As}/\text{GaAs} \) single QW details are \( L_z = 10 \) nm, \( x = 0.2 \).
Fig. 5.6. Schematic diagram showing an as-grown section of an InGaAs/GaAs QW structure flanked by disordered areas on either side. Lateral confinement of photons is possible in the as-grown section for light propagating parallel to the QW layer.
Fig. 5.7. Wavelength spectra for TE polarisation of the lateral refractive index step, \( \Delta n_r = n_r(L_d = 0) - n_r(L_d) \), for various values of interdiffusion length \( L_d \). The as-grown In\(_x\)Ga\(_{1-x}\)As/GaAs single QW details are (a) \( L_z = 5 \) nm, \( x = 0.2 \), and (b) \( L_z = 5 \) nm, \( x = 0.3 \).
lateral confinement of light propagating parallel to the QW layer in an InGaAs/GaAs QW structure is shown in Fig. 5.6.

The TE polarisation refractive index step for the narrower well ($L_z = 5\text{ nm}$, $x = 0.2$), is shown in Fig. 5.7(a). $\Delta n_{\tau}$ for the same $L_d/L_z$ ratio, at wavelengths immediately above the $L_d = 0$ exciton edge, $\lambda = 1.05\mu m$, is larger for the narrower well. This is due to the fact that for the $L_z = 5\text{ nm}$ wells the refractive index rises more sharply to its peak value than for the $L_z = 10\text{ nm}$, resulting in a larger index step for the narrower wells. At longer wavelengths, $\lambda \approx 1.2\mu m$, $\Delta n_{\tau}$ for the same $L_d/L_z$ ratio for the two wells tend to converge. The $\Delta n_{\tau}$ wavelength spectra for the QW structure with as-grown $L_z = 5\text{ nm}$, $x = 0.3$, see Fig. 5.7(b), show that keeping the well width constant and changing the In content also significantly changes $\Delta n_{\tau}$. For the same $L_d/L_z$ ratio, $\Delta n_{\tau}$ at wavelengths immediately above the exciton edge is larger for $x = 0.3$ than for $x = 0.2$, and remains larger even at longer wavelengths. For $x = 0.3$, the ground state C-HH transition energy for the as-grown well is smaller than that for $x = 0.2$, while the strain in the well is larger. Consequently, the combined effects of disordering and strain on the ground state C-HH transition energy are more pronounced in the higher In content well, thereby resulting in an increased $\Delta n_{\tau}$. This is particularly evident as interdiffusion increases. It can be seen from the above that $\Delta n_{\tau}$ is sensitive to both the In content as well as to the as-grown well width, and that its value increases with the extent of disordering.

5.4. Birefringence

The birefringence is defined here as the difference between the TE polarisation and the TM polarisation refractive index of the QW structure. Fig. 5.8 shows the birefringence, $n_{r}^{\text{TE}} - n_{r}^{\text{TM}}$, for the InGaAs/GaAs single QW with $L_z = 10\text{ nm}$, $x = 0.2$. 

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Fig. 5.8. Birefringence spectra for different values of interdiffusion length $L_d$: $L_d = 0$ (solid line), $L_d = 2$ nm (dot-dashed line), $L_d = 4$ nm (dashed line). The as-grown In$_x$Ga$_{1-x}$As/GaAs single QW details are $L_z = 10$ nm, $x = 0.2$. 
The birefringence is large for the wavelength range $0.87 \, \mu m < \lambda < 1.01 \, \mu m$, which is the range between the barrier band edge and the strained $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$ band edge, where the QW subband states are situated. The birefringence outside this range is small ($\approx 0.002$), so that at the longer wavelengths the refractive index is polarization independent. A small birefringence is desirable in waveguide applications, while a large birefringence is desirable in modulator applications. As can be seen from Fig. 5.8, birefringence rises to a positive peak at the QW band edge ($\lambda = 1.01 \, \mu m$, for $L_d = 0 \, \text{nm}$) since at this wavelength the TE polarization $n_e$ dominated by the HH exciton band edge, reaches a peak. The TM polarization $n_e$, which is dominated by the LH exciton band edge, reaches a peak at $\lambda = 0.95 \, \mu m$ so that around this wavelength the birefringence exhibits a negative peak.

The birefringence at the QW band edge wavelength for the $\text{InGaAs/GaAs}$ QW structure is larger than the birefringence at its QW band edge wavelength for an $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As/GaAs}$ QW with $L_d = 10 \, \text{nm}$. This is in large measure due to the strain present in the $\text{InGaAs}$ layer, which results in a large separation between the ground state HH and LH subbands, so that the wavelength separation between the TE polarization band edge $n_e$ peak and the TM polarization band edge $n_e$ peak is much larger for the strained QW than for the lattice-matched QW.

With interdiffusion, the birefringence of the QW structure decreases and the wavelength range where the birefringence is large also decreases (from $0.14 \, \mu m$ to $0.09 \, \mu m$ as $L_d$ increases from 0 to 4 nm) since the QW band edge moves towards the barrier band edge as a result of interdiffusion. The wavelength region where the refractive index is polarization independent thus increases with interdiffusion. The birefringence decreases with interdiffusion since the HH exciton band edge transition energy increases more than the LH exciton band edge transition energy. This difference
Fig. 5.9. Birefringence spectra for different values of interdiffusion length $L_d$, for single In$_x$Ga$_{1-x}$As/GaAs single QW structures with as-grown details: (a) $L_z = 5$ nm, $x = 0.2$, and (b) $L_z = 5$ nm, $x = 0.3$. $L_d = 0$ (solid line), $L_d = 1$ nm (dot-dashed line), $L_d = 2$ nm (dashed line).
in the change in transition energies is more pronounced in the compressively strained InGaAs/GaAs because of the shallow LH confinement profile that results from the strain-induced HH-LH band edge splitting. This leads to a larger reduction of \( n_r \) for the TE than the TM polarisation, resulting in a reduction of the birefringence. The birefringence decrease in going from \( L_d = 2 \text{ nm} \) to \( 4 \text{ nm} \) is larger than that exhibited in going from \( L_d = 0 \) to \( 2 \text{ nm} \), again as a result of the correspondingly higher HH exciton band edge transition energy increase already noted above.

The \( L_g = 5 \text{ nm}, x = 0.2 \) QW exhibits a larger birefringence (approximately twice at the peaks, Fig. 5.9) than the \( L_g = 10 \text{ nm}, x = 0.2 \) QW, for corresponding \( L_d/L_g \) ratios, in the QW band edge to barrier band edge wavelength range. This is mainly due to the sharper \( n_r \) peaks observed in the case of the narrower well. Calculations also show that the \( L_g = 5 \text{ nm}, x = 0.3 \) QW birefringence is somewhat larger than that for the \( L_g = 5 \text{ nm}, x = 0.2 \) QW. In this second case, the increased birefringence of the \( L_g = 5 \text{ nm}, x = 0.3 \) QW is mainly attributable to a larger strain-induced HH1-LH1 band edge separation, (110 meV for \( x = 0.3 \) against 73 meV for \( x = 0.2 \)), which shifts the \( n_r \) peak of the TM polarisation further away from the \( n_r \) peak of the TE case so that \( n_r^{\text{TE}} - n_r^{\text{TM}} \) at the TE polarisation QW band edge wavelength increases. Birefringence in \( \text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs} \) structures is thus sensitive to both well width and In composition variations, for wavelengths close to the QW band edge. For longer wavelengths the birefringence tends to \( \approx 0.002 \) for all the QW structures considered, indicating a polarisation independent refractive index at these wavelengths.

5.5. Summary

The refractive index spectra of disordered, strained InGaAs/GaAs single QWs, for both TE and TM polarisations have been calculated for the wavelength range 0.87 \( \mu \text{m} \)
to 2 μm, using the complex dielectric function, taking into consideration the contributions from the Γ, X and L valleys of the Brillouin zone. The results show that for wavelengths > 1 μm the refractive index decreases as the extent of disordering increases, resulting in a positive refractive index step with respect to the as-grown, or the less disordered, structures. This lateral refractive index step is larger when the confining regions are more extensively disordered. Calculations also show that the positive refractive index step increases with decreasing well widths, or with increasing In content. At the longer wavelengths the refractive index step is more sensitive to the In content than to the width of the QW, partly as a result of the strain in the InGaAs layer.

The QW structure exhibits a large birefringence in the QW band edge to barrier band edge wavelength range, which decreases with interdiffusion. Outside this range the birefringence is ≤ 0.002, indicating that the refractive index is polarisation independent. Interdiffusion increases this range of polarisation independent refractive index. Results obtained indicate that birefringence in InGaAs/GaAs QW structures is sensitive to both QW widths and to the In content.

Selective area QW disordering is thus a potentially important process in providing strong lateral photon confinement also in strained QW structures. The above results can be of interest in waveguide and modulator applications at fibre optic communication wavelengths, particularly in the context of monolithic integration.
5.6. References


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Chapter 6

APPLICATION OF AN ELECTRIC FIELD TO DISORDERED
InGaAs/GaAs SINGLE QUANTUM WELLS

Quantum well (QW) optical modulators have been the focus of much attention for optical switching and computing applications. The optical modulation is due to the quantum-confined Stark effect (QCSE), which is unique to QW structures, and which describes the change in the absorption properties of QW structures when an electric field is applied across the structure. In this chapter the application of an electric field to disordered InGaAs/GaAs single QWs is discussed. The effects of the electric field, applied perpendicular to the QW layer, on the subband states in the disordered, strained QWs are first presented. The effects of disordering on the quantum-confined Stark shift is then determined for various stages of interdiffusion, and the possibility of enhanced electroabsorption in disordered InGaAs/GaAs QWs is briefly considered.

6.1. Introduction

When an electric field is applied perpendicular to the QW layer the carrier confinement profiles are altered, and the ground state energies of the carriers are shifted, resulting in a reduced ground state transition energy. The electric field does not destroy the enhanced absorption due to the excitons, as happens in bulk semiconductors, but results in a shift of the room temperature exciton absorption to longer wavelengths. This phenomenon is the so-called QCSE, and has been observed in several III-V material systems including AlGaAs/GaAs, and InGaAs/GaAs strained QW structures.
Light, of appropriate wavelength, propagating in the QW structure can be modulated by this change in the fundamental absorption edge with applied electric field.

The QCSE is investigated experimentally by placing the QW structure in the intrinsic region of a p-i-n diode, and applying the electric field so that the diode is reversed biased.\(^6\) InGaAs/GaAs QW optical modulators and self-electro-optic-effect devices,\(^6\,5\,6\,6\) where light propagates perpendicular to the QW layer, have been studied. More recently InGaAs/GaAs QW waveguide modulators, where light propagates parallel to the QW layer, have also been investigated.\(^6\,7\) Such modulators are particularly interesting for monolithic integration with low threshold strained-layer laser diodes.\(^6\,8\)

For high device performance, such as high on/off ratio and a low operation voltage, a limited decrease of the exciton oscillator strength and a large Stark shift of excitons by the external electric field are desired. Non-square confinement profiles have been proposed to realise these requirements.\(^6\,9\) The interdiffusion induced graded profile that results from disordering is investigated here as a possible candidate for improved device properties.

### 6.2. Quasi-Bound States in Disordered, Compressively Strained Quantum Wells

For any finite value of electric field applied perpendicular to the QW layer there are no true bound eigenstates, but rather quasi-bound states. For small enough electric fields, and large enough barrier heights, the instability of the eigenlevel of the quasi-bound states due to tunnelling is very narrow (less than 0.001 meV wide), except for high-energy subbands.\(^6\,10\) For larger fields it is necessary to impose arbitrary boundary conditions which preclude exactness and necessitate examination of the QW eigenstate outside the well to determine the validity of the result.\(^6\,11\)
The quasi-bound states are determined by solving Schrödinger’s equation (eq. (2) of chapter 3) for a QW of width $L_z$ in an applied electric field, as illustrated in Fig. 6.1, and which is given by:

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left[ \frac{1}{m^*_n(z)} \frac{d\chi_n(z)}{dz} \right] + [U_p(z) + U_r(z)]\chi_n(z) = E_n \chi_n(z) \tag{1}$$

where $z$ is the growth direction, and $U_p(z)$ is the tilted potential arising from the applied electric field $F$:

$$U_p(z) = \pm eFz \tag{2}$$

where $e$ is the electronic charge. As with many numerical approaches, the algorithm can only be applied over a finite region of space, necessitating arbitrary boundaries and boundary conditions on the solution. For states that are sufficiently quasi-bound (with small enough linewidths so that the state can be considered to be bound), then if the boundary is sufficiently far away from the QW, it should have no effect on the eigenstates. This can be used as a reasonable criteria for having a well-defined quasi-bound state. In the numerical calculations a boundary is placed at $z = -L_B = -4L_z$ and at $z = +L_B = +4L_z$, with $z = 0$ being the QW centre, see Fig. 6.1. It is assumed here that the arbitrary barrier at $z = \pm L_B$ has infinite height and that the wave function must be zero at the boundaries. The boundaries are then moved by a few percent and the eigenstates obtained again. If they do not vary by more than 0.01 meV then it is safe to assume that the eigenstate is a well-defined eigenstate (less than 0.01 meV in width). For the as-grown InGaAs/GaAs structure considered here, where the barrier heights are about 100 meV, well-defined quasi-bound states are obtained for the ground state for moderate electric fields (50-90 kV/cm). For the excited states in the as-grown wells and for the ground states in disordered wells ($L_d \approx 2$ nm), the assumption...
Fig. 6.1. An as-grown and disordered QW under the influence of an external electric field. The as-grown well width is $L_x$. Arbitrary potential boundaries with infinite height are shown at $-L_B$ and $+L_B$. 

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of quasi-bound states breaks down at small electric fields (< 50 kV/cm). For large enough electric fields, the assumption of quasi-bound states becomes meaningless for both the ground and excited states as the particle becomes unbound and tunnels out of the well.

The carrier confinement profiles under the influence of an external electric field for an In$_x$Ga$_{1-x}$As/GaAs single QW with $x = 0.2$ and $L_z = 10$ nm are shown in Fig. 6.2 to Fig. 6.4, for $L_d = 0, 1,$ and $3$ nm, respectively, for $F = 0, 20,$ and $40$ kV/cm. Note that the energy gap between the electron (C) and heavy hole (HH) confinement profiles is arbitrary, and that the zero of energy for the electron confinement profile is taken at the well centre $z = 0$, while the zero of energy for the hole confinement profiles is taken as the HH confinement profile energy at $z = 0$. As already noted, disordering in InGaAs/GaAs QWs leads to a nonlinear confinement profile and a decrease in the QW depth. Applying an electric field to the disordered QW produces an asymmetric, nonlinear confinement profile due to the lowering of the barrier on one side, and further reduces the QW depth.

The effect of the compressive strain in the InGaAs layer is immediately evident in the very shallow light hole (LH) confinement profile that results, for all cases of $L_d$ shown for $F = 0$ kV/cm, due to the HH-LH band edge splitting. In the absence of an electric field, the LH wave function is only weakly confined and penetrates significantly into the barrier, as can be seen from Fig. 6.5, where the ground state electron, heavy hole, and light hole wave functions squared, representing the carrier probability density, $|\chi_\alpha(z)|^2$, for the as-grown QW are shown. This confirms the reasonableness of neglecting the effect of the LH subband on the HH subband for small wave numbers $k_{||}$ in the plane of the QW. As soon as an electric field is applied the LH starts to tunnel out. This can be seen in Fig. 6.5(d) which shows the LH wave function at $F = 3$ kV/cm. The confinement profiles in Fig. 6.2 to Fig. 6.4 illustrate another effect
Fig. 6.2. Electron (C), heavy hole (HH), and light hole (LH) confinement profiles for an as-grown $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QW with $L_z = 10$ nm, and $x = 0.2$, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm.
Fig. 6.3. Electron (C), heavy hole (HH), and light hole (LH) confinement profiles for a disordered InGaAs/GaAs QW with $L_d = 1$ nm, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm.
Fig. 6.4. Electron (C), heavy hole (HH), and light hole (LH) confinement profiles for a disordered InGaAs/GaAs QW with $L_d = 3$ nm, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm.
Fig. 6.5. Electron (solid), heavy hole (dot-dash), and light hole (dotted) ground state wave functions for the as-grown InGaAs/GaAs QW for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm. The dashed lines indicate the boundaries of the as-grown QW. (d) The LH wave function at $F = 3$ kV/cm, indicating tunnelling out of the well.
of the compressive strain in the QW, already noted in chapter 3. Although a 70:30 conduction-to-valence band offset ratio is used, nearly equal barrier heights result for the conduction and HH bands, because of the compressive strain. This differs from lattice-matched AlGaAs/GaAs and can give rise to a contrasting effect when an electric field is applied, as will be discussed below.

Fig. 6.5(a)-(c) show the effect of the electric field on the electron and heavy hole ground state wave functions for $L_d = 0$. The boundaries of the QW are depicted by the dashed lines. The shift of the electron eigenfunction to the right and of the heavy hole eigenfunction to the left, as a function of the electric field, and the increase in penetration of the wave functions out of the well are clearly evident. In every case, the overlap between the electron and heavy hole wave functions is reduced. States with lower energies in the confining wells are affected more by applied fields than those with higher energies. Consequently, HH wave functions are affected more than the electron wave functions. This can be seen by comparing Fig. 6.5(a) and (c). The wave functions for the ground state eigenstates for $L_d = 1$ nm and $L_d = 3$ nm are shown in Fig. 6.6 and Fig. 6.7, respectively. For $L_d = 1$ nm, the states are well confined at the highest applied field shown, $F = 40 \text{ kV/cm}$. For $L_d = 3$ nm, however, tunnelling out of the ground state electron can be seen at $F = 40 \text{ kV/cm}$ since the confinement profiles, shown in Fig. 6.4(c), are now quite shallow ($\approx 20 \text{ meV}$).

As interdiffusion proceeds, the value of the electric field at which tunnelling out of the particle starts to be seen diminishes. In the case of the ground state electron, tunnelling out starts at $F = 60 \text{ kV/cm}$, $50 \text{ kV/cm}$, and $35 \text{ kV/cm}$ for $L_d = 0$ nm, 1 nm, and 3 nm, respectively, while the ground state HH starts to tunnel out at $F = 105 \text{ kV/cm}$, $90 \text{ kV/cm}$, and $50 \text{ kV/cm}$, for $L_d = 0$ nm, 1 nm, and 3 nm, respectively, as shown in Fig. 6.8 and Fig. 6.9. It can be seen from these results that for every value of $L_d$, the
applied field at which the ground state electron starts to tunnel out is lower than the
applied field at which the ground state HH starts to tunnel out, with the difference
decreasing with interdiffusion. This is in marked contrast to the lattice-matched
AlGaAs/GaAs QW system. Calculations for an Al$_{0.3}$Ga$_{0.7}$As/GaAs QW with an as-grown
$L_z = 10$ nm show that the ground state electron starts to tunnel out at $F = 205$ kV/cm,
75 kV/cm, and 50 kV/cm for $L_d = 0$ nm, 4 nm, and 6 nm, respectively, while the
corresponding applied field values at which the ground state HH starts to tunnel out are
$F = 170$ kV/cm, 50 kV/cm, and 25 kV/cm, respectively. A 70:30 conduction-to-valence
band offset ratio\textsuperscript{6,13} is used in these calculations and the resulting depths of the
conduction and hole confinement profiles for the lattice-matched QW, for the as-grown
case, are 300 meV and 120 meV, respectively. Due to the compressive strain, the depth
of the electron and HH confinement profiles is nearly the same, as noted above, and with
a suitable applied field, a situation can be engineered where the absorption of a photon
results in a transition from the ground state in the HH band to the ground state in the
conduction band, where the electron can then tunnel out in the presence of this field.
This effect can be of interest in device applications.

Examples of HH excited state wave functions for the as-grown QW are shown in
Fig. 6.10. It can be seen that up to $F = 40$ kV/cm the first excited state is well confined.
The higher excited states, however, begin to tunnel out at lower electric fields,
Fig. 6.10(d). Fig. 6.11 shows the HH first excited state wave functions for $L_d = 1$ nm.
Disordering again lowers the value of the electric field at which the wave functions start
to tunnel out. The HH first excited state tunnels out at $F = 65$ kV/cm, 45 kV/cm,
(Fig. 6.11(d)), and 35 kV/cm, as $L_d$ increases from 0 nm, to 1 nm, to 3 nm, respectively.
The assumption of quasi-bound states thus breaks down at smaller electric fields as the
extent of disordering increases.
Fig. 6.6. Electron (solid), heavy hole (dot-dash), and light hole (dotted) ground state wave functions for disordered InGaAs/GaAs QW with $L_d = 1$ nm, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm. The dashed lines indicate the boundaries of the as-grown QW.
Fig. 6.7. Electron (solid), heavy hole (dot-dash), and light hole (dotted) ground state wave functions for disordered InGaAs/GaAs QW with $L_d = 3$ nm, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm. The dashed lines indicate the boundaries of the as-grown QW. Tunnelling out of the electron wave function can be seen in (c).
Fig. 6.8. Electron (solid) and HH (dot-dash) ground state wave functions plotted for the electric field at which the electron starts to tunnel out of the QW, for (a) $L_d = 0$ nm, (b) $L_d = 1$ nm, and (c) $L_d = 3$ nm. The dashed lines indicate the boundaries of the as-grown $\text{In}_{0.2}\text{Ga}_{0.8}\text{As/GaAs}$ QW.
Fig. 6.9. Electron (solid) and HH (dot-dash) ground state wave functions plotted for the electric field at which the HH starts to tunnel out of the QW, for (a) \( L_d = 0 \) nm, (b) \( L_d = 1 \) nm, and (c) \( L_d = 3 \) nm. The dashed lines indicate the boundaries of the as-grown \( \text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs} \) QW.
Fig. 6.10. Heavy hole first excited state wave function for the as-grown QW, for applied fields (a) \( F = 0 \) kV/cm, (b) \( F = 20 \) kV/cm, and (c) \( F = 40 \) kV/cm. (d) The heavy hole second excited state wave function tunnels out of the well for \( F = 25 \) kV/cm. The dashed lines indicate the boundaries of the as-grown QW.
Fig. 6.11. Heavy hole first excited state wave function for $L_d = 1$ nm, for applied fields (a) $F = 0$ kV/cm, (b) $F = 20$ kV/cm, and (c) $F = 40$ kV/cm. (d) The heavy hole first excited state wave function tunnels out of the well for $F = 45$ kV/cm. The dashed lines indicate the boundaries of the as-grown QW.
6.3. Effects of Disordering on the Quantum-Confined Stark Shift

The electron and hole subbands are considered assuming the conduction band to be parabolic and that the LH subband shift due to the strain-induced HH-LH band edge splitting is large enough to neglect valence band mixing. The subbands are determined by solving eq. (1), according to the method described above, following a scheme developed by Bloss. These subbands are then used to calculate the heavy-hole related 1S exciton binding energies and wave functions by a perturbative-variational method, as detailed in chapter 4. Since the LH wave function is only weakly confined in the absence of an electric field, and tunnels out immediately under the influence of an electric field, it is assumed that for the compressively strained InGaAs/GaAs QWs considered here, subsequent calculations may be safely carried out in a model which takes into account just the conduction and heavy hole subbands. Numerical results are calculated for various values of interdiffusion. An error function distribution is assumed after disordering, and the extent of interdiffusion is characterized by the interdiffusion length $L_d$.

Fig. 6.12 shows the HH exciton binding energy change with applied electric field, defined as $E_b(F) - E_b(F = 0)$, for various values of $L_d$. The exciton binding energy decreases with increasing applied field strength in all cases. The applied field causes the electrons and heavy holes to move to opposite sides of the well, and this makes the exciton less two-dimensional, thereby reducing the binding energy. In the initial stages of interdiffusion ($L_d = 1$ nm) the exciton binding energy shift decreases slightly and then increases to a value larger than the as-grown case, showing a significantly larger value for $L_d = 3$ nm. This reflects the changing effective width of the confinement profile, as modified by disordering, strain and applied field, experienced by the electron and HH ground states, shown in Fig. 6.2 to Fig. 6.4.
Fig. 6.12. The change in exciton binding energy with applied electric field for an In$_{0.2}$Ga$_{0.8}$As/GaAs single QW with an as-grown $L_z = 10$ nm, for various values of interdiffusion: $L_d = 0$ (solid line), $L_d = 1$ nm, 2 nm, and 3 nm.
Fig. 6.13 shows the exciton Stark shift energy for the HH related transitions with applied electric field, for various values of $L_d$. It can be seen that the Stark shift is much larger in magnitude than the exciton binding energy shift shown in Fig. 6.12, indicating that the major contribution to the Stark shift comes from the ground state (C1-HH1) transition energy. In a manner similar to the exciton binding energy shift, the Stark shift for $L_d = 1$ nm is slightly less than the as-grown case, while it is larger than the as-grown case for $L_d > 2$ nm. The results show that for a sufficiently large value of $L_d$ the exciton Stark shift in the disordered QW is greater than in the as-grown QW case. The applied field lowers the ground state subbands, and thus the ground state transition energy, to a greater extent in the disordered QW ($L_d \geq 2$ nm, in this case), and the average of the spatially dependent effective masses over the well region is larger in the disordered QW, as a result of the increasing effective masses with increasing distance from the well centre. The increase in Stark shift in the disordered QW is similar in trend to results calculated for a graded-gap QW structure. Since for $L_d = 1$ nm the Stark shift is less than that for $L_d = 0$ nm, a higher operational voltage would be required to obtain a desired Stark shift. For $L_d = 3$ nm, the Stark shift at 30 kV/cm is enhanced by a factor of 65% over the as-grown QW case. This enhancement could be the basis of improved device performance in electroabsorption modulators which can be driven with a low operational voltage and possess a high on/off ratio. The Stark shift values for the as-grown QW, compare favourably with reported calculated values for an InGaAs/GaAs QW structure with similar barrier heights of 100 meV. It should be noted that the Stark shift values determined here for the strained, disordered InGaAs/GaAs QW are comparable to Stark shift values obtained when considering interdiffusion in an Al$_{0.3}$Ga$_{0.7}$As/GaAs QW with $L_z = 10$ nm, even though in the latter case the conduction and hole barrier heights, for $L_d = 0$ nm, are 300 meV and 120 meV, respectively.
Fig. 6.13. Quantum-confined Stark shift with applied electric field for an In_{0.2}Ga_{0.8}As/GaAs single QW, with an as-grown $L_x = 10$ nm, for various values of interdiffusion length $L_d$. 
6.4. Electroabsorption in Disordered InGaAs/GaAs Quantum Wells

Waveguide electroabsorption is considered here, with the light propagating along the plane of the QW layer. The absorption coefficient is calculated for the band edge \( \Gamma \) region of the Brillouin zone taking into consideration only HH to conduction transitions, in view of the effects of the compressive strain on the LH subband, as discussed above. Results are presented for the TE polarisation absorption coefficient determined by taking into consideration the 1S exciton, and all the bound states, including the 2D enhancement Sommerfeld factor, which are given by:

\[
\alpha_{\text{ud}}(\omega) = \frac{e^2 \mu_{||}^* \omega}{6 \varepsilon_0 c n_{||} m_e^* E_{CV}^2 L_z} \sum_{\mu \lambda} \langle \chi_{\text{HH}} | \chi_{\text{HH}} \rangle |^2 \int_{0}^{\infty} \mathcal{F}(E) S(\omega) \mathcal{F}(E_{\mu \lambda} - E_{\text{HH}}) dE
\]

Where

\[
\mathcal{F}(E) = \frac{P(E) S(\omega) S(E_{\mu \lambda} - E_{\text{HH}})}{E_{\text{HH}}}
\]

and

\[
\alpha_{\text{ex}}(\omega) = \frac{e^2 \gamma^2 \varphi \omega}{3 \varepsilon_0 c n_{||} m_e^* E_{CV}^2 L_z} \sum_{\mu \lambda} \langle \chi_{\text{CL}} | \chi_{\text{HL}} \rangle |^2 \int_{0}^{\infty} \mathcal{F}(E_{\text{ex}}) S(\omega) \mathcal{F}(E_{\text{exc}} - E_{\text{ex}}) dE
\]

where \( \varphi \) is the polarisation factor at the band edge, with \( \varphi_{\text{HH}} = 3/2 \) (HH), 1/2 (LH) and \( \varphi_{\text{HL}} = 0 \) (HH), 2 (LH); \( S \) is the Sommerfeld enhancement factor; \( \mathcal{F} \) is the Lorentzian broadening factor with a half width half maximum \( \Gamma_w \); \( \bar{M}_o = \bar{E}_o (\bar{E}_o + \bar{A}_o)/3 \); \( \bar{E}_o \) is the interdiffusion induced bandgap at the QW centre; \( E_p, E_q, \) and \( E_{\text{exc}} \) are the electron subband energy, hole subband energy, and exciton transition energy, respectively; \( E_{CV} = E_p + E_{\text{CL}} + E_{\text{VL}} \); \( \chi_{\text{CL}}, \chi_{\text{CV}}, \chi_{\text{IS}} \) are the envelope wave functions for the electrons, the holes, and the exciton, respectively; \( \varepsilon_0 \) is the permittivity of free space; \( \mu_{||}^* \) is the in-plane reduced mass; \( m_e^* \) is the electron effective mass along the quantization axis \( z \); and \( L_z \) is the as-grown QW width centred at \( z = 0 \). The values of
the material parameters used are as indicated earlier in chapter 3 and chapter 4. In this first analysis, the contributions from continuum states above the barrier gap have not been considered. This should only have a small effect on the electroabsorption spectrum near the fundamental absorption edge.

The room temperature absorption coefficient spectra for TE polarisation for an as-grown QW and for the disordered QW with L_d = 3 nm is shown in Fig. 6.14, for various values of applied field. The exciton peak shifts to longer wavelengths with increasing applied field, reflecting the QCSE, at the same time decreasing in value. As already evidenced in Fig. 6.5 to Fig. 6.7 the applied field pulls apart the electron and HH wave functions thereby reducing the electron-HH wave function overlap, and thus the exciton peak. A similar trend in the behaviour of the exciton peak at the fundamental absorption edge is observed in the disordered QW. The decrease in the exciton peak for similar values of applied field is larger for the disordered QW than for the as-grown QW. In the disordered QW the electron and HH wave functions are less strongly confined and show a larger penetration out of the well. At the same time the electric field pulls apart the two wave functions. Consequently, the electron-HH wave function overlap, and therefore the exciton peak, is reduced to a greater extent.

Fig. 6.15 shows the change in the TE polarisation absorption coefficient due to the application of an electric field, for wavelengths around the fundamental absorption edge, for L_d = 0 nm and 3 nm, respectively. This change in electroabsorption is defined as \( \Delta \alpha = \alpha(F) - \alpha(F = 0) \). For the as-grown QW electric fields up to 40 kV/cm are considered, while for the disordered QW electric fields up to 30 kV/cm only are considered since tunnelling out can be observed at 40 kV/cm for L_d = 3 nm. It can be seen that a similar maximum value of \( \Delta \alpha \) results near the respective fundamental absorption edge in the two cases L_d = 0 nm with F = 40 kV/cm, and L_d = 3 nm with
Fig. 6.14. Absorption coefficient wavelength spectra for TE polarisation for an In$_{0.2}$Ga$_{0.8}$As/GaAs single QW with $L_z = 10$ nm, for various values of applied field: $F = 0$ kV/cm (solid), 10 kV/cm (long dash), 20 kV/cm (dotted), 30 kV/cm (dot-dash), and 40 kV/cm (short dash), for (a) $L_d = 0$, and (b) $L_d = 3$ nm.
Fig. 6.15. Change in absorption coefficient for TE polarisation, $\Delta \alpha$, with applied field, for an In$_{0.2}$Ga$_{0.8}$As/GaAs single QW with $L_z = 10$ nm, where $\Delta \alpha = \alpha(F) - \alpha(F=0)$, for various values of applied field: $F = 10\, \text{kV/cm}$ (long-dash), $20\, \text{kV/cm}$ (dotted), $30\, \text{kV/cm}$ (dot-dash), and $40\, \text{kV/cm}$ (short-dash), for (a) $L_d = 0$, and (b) $L_d = 3$ nm.
F = 30 kV/cm. This implies that the same maximum \( \Delta \alpha \) can be achieved in the disordered structure at a lower operational voltage. This enhancement in electroabsorption can be seen also by comparing the maximum \( \Delta \alpha \) for the as-grown and disordered QW at the same applied field. At F = 30 kV/cm, the maximum \( \Delta \alpha \) for the disordered QW is 30% larger than that of the as-grown QW. Ideally this implies an improved on/off ratio for the same waveguide modulator length or a reduced device length for the same on/off ratio, the latter being particularly attractive in high speed optoelectronic circuit applications.

The above calculations have also been carried out to investigate the effects of disordering of an In_{0.3}Ga_{0.7}As/GaAs single QW with \( L_z = 5 \) nm. In this QW structure the confinement profiles of the as-grown QW are narrower and deeper. It is found in this case that for the disordered QW with \( L_d = 2 \) nm the Stark shift at 50 kV/cm is three times the value for \( L_d = 0 \). This is reflected in the change with applied field of the \( \Delta \alpha \) values near the fundamental absorption edge, shown in Fig. 6.16. The maximum value of \( \Delta \alpha \) for the disordered QW at F = 50 kV/cm is 100% higher than the maximum value of \( \Delta \alpha \) for the as-grown QW at F = 70 kV/cm. By comparing Figs. 6.15(a) and 6.16(a) it can be seen that although a higher electric field can be applied (before particle tunnelling starts to be seen) for the \( x = 0.3, L_z = 5 \) nm, \( L_d = 0 \) QW structure, the maximum value of \( \Delta \alpha \), at F = 70 kV/cm, is less than the maximum value of \( \Delta \alpha \), at F = 40 kV/cm, for the \( x = 0.2, L_z = 10 \) nm, \( L_d = 0 \) QW. This is due to the fact that the ground state subbands for the former structure are at a higher level than in the latter structure, so that they are less affected by the applied field. However, for the disordered QWs, the maximum value of \( \Delta \alpha \) for the \( x = 0.3, L_z = 5 \) nm, \( L_d = 2 \) nm QW at F = 50 kV/cm, Fig. 6.16(b), is 67% larger than the value for \( x = 0.2, L_z = 10 \) nm, \( L_d = 3 \) nm QW at F = 30 kV/cm, Fig. 6.15(b). Thus although for the as-grown QWs a
Fig. 6.16. Change in absorption coefficient for TE polarisation, $\Delta \alpha$, with applied field, for an In$_{0.3}$Ga$_{0.7}$As/GaAs single QW with $L_z = 5$ nm, where $\Delta \alpha = \alpha(F) - \alpha(F=0)$, for various values of applied field: $F = 10$ kV/cm (long-dash), 30 kV/cm (dotted), 50 kV/cm (dot-dash), and 70 kV/cm (short dash), for (a) $L_d = 0$, and (b) $L_d = 3$ nm.
smaller maximum $\Delta\alpha$ results for the $x = 0.3$, $L_z = 5$ nm QW, disordering can reverse the situation at the higher electric fields that can be applied before tunnelling of particles is in evidence. These results confirm that significant enhancement in electroabsorption can be achieved near the fundamental absorption edge around 1 $\mu$m, by disordering strained InGaAs/GaAs QW structures, indicating the potential of improving modulator performance by lowering the operational voltage and increasing the on/off ratio. The results also provide another illustration of the flexibility that disordered, strained QW structures can offer in designing QW structures for enhanced device performance.

6.5. Summary

The application of an external electric field to disordered InGaAs/GaAs single QWs is discussed. The effects of the electric field, applied perpendicular to the QW layer, on the carrier confinement profiles and subband states in the compressively strained, disordered QWs are first presented. The effects of disordering on the exciton binding energy change with applied field, and on the quantum-confined Stark shift with applied field, are determined for different stages of interdiffusion. These results are used to calculate changes in electroabsorption that result from disordering of strained QWs.

The carrier confinement profiles of the disordered, strained QWs under the influence of an applied field exhibit an asymmetric, nonlinear profile due to the lowering of the barrier on one side by the electric field and the error function compositional distribution in the QW after interdiffusion. Well defined quasi-bound states are obtained for the ground state for moderate electric fields in the as-grown QW case, while for excited states the assumption of quasi-bound states breaks down at smaller electric fields. As interdiffusion proceeds the value of applied field at which tunnelling out of a particle starts to be seen gets smaller.
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The compressive strain in the QW results in a very shallow LH confinement profile, leading to weak LH confinement, and when an electric field is applied the LH is no longer confined and tunnels out of the well. The compressive strain also leads to nearly equal conduction and HH barrier heights in both the as-grown and disordered QWs. As a result, the ground state electron starts to tunnel out of the well at values of electric field that are smaller than those for the ground state HH. Thus, under the action of an applied field, the absorption of a photon with the appropriate energy can result in a transition from the ground state in the HH band to the ground state in the conduction band, where the particle can then tunnel out in the presence of this field. This effect may be of interest for device applications. In contrast, in lattice-matched AlGaAs/GaAs QWs, the HH ground state starts to tunnel out at values of electric field that are smaller than those of the electron, because of the pronounced difference between the conduction and valence band barrier heights.

The change in the HH exciton binding energy with applied field is determined for various values of $L_d$. The exciton binding energy decreases with increasing applied field strength in all cases. The exciton binding energy shift decreases slightly in the initial stages of interdiffusion ($L_d \sim 1$ nm) and then increases to a value larger than the as-grown case, showing a significantly larger value for $L_d = 3$ nm. The quantum-confined Stark shift with applied electric field is also calculated for various values of $L_d$. The results show that for a sufficiently large value of $L_d$ the exciton Stark shift in the disordered QW is greater than in the as-grown QW. For $L_d = 3$ nm the Stark shift at 30 kV/cm is enhanced by a factor of 65% over the as-grown QW case.

The absorption coefficient spectra for TE polarisation for an as-grown QW and for the disordered QW with $L_d = 3$ nm are determined around the fundamental absorption edge. In both cases the exciton peak shifts to longer wavelengths with increasing applied
field, as a result of the QCSE, and at the same time decreases in value, but the effects are more pronounced in the disordered QW. The change in electroabsorption is, in fact, larger in the disordered QW than in the as-grown QW for the same applied field. At $F = 30 \text{kV/cm}$, the maximum $\Delta \alpha$ for the disordered QW is 30% larger than that of the as-grown QW. This implies that in disordered InGaAs/GaAs QWs an improved on/off ratio or reduced device length in waveguide modulators could be achieved for wavelengths around $1 \mu\text{m}$.

Similar calculations for an $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QW with $x = 0.3$, $L_g = 5 \text{ nm}$ show that whereas the maximum $\Delta \alpha$, at $L_d = 0$, for this structure is less than that for the $x = 0.2$, $L_g = 10 \text{ nm}$ QW, disordering can reverse the situation, with the disordered $x = 0.3$, $L_d = 2 \text{ nm}$ QW having a higher maximum $\Delta \alpha$ near the fundamental absorption edge than the disordered $x = 0.2$, $L_d = 3 \text{ nm}$ QW. These results provide another example of the flexibility that disordered, strained QW structures can provide in optimising device performance, due to the lifting of the lattice-matching constraint.
6.6. References


Epitaxial layers of InGaAs can be grown not only on GaAs substrates but also on InP substrates. Lattice-matched In$_{0.53}$Ga$_{0.47}$As/InP QW structures are of considerable interest in photonic applications, such as waveguides and modulators, since they enable device operation in the $1.3 \mu m$ to $1.55 \mu m$ wavelength range, which is of importance for optical communication systems. Selective area disordering of In$_{0.53}$As$_{0.47}$As/InP QWs is being actively investigated, with special emphasis on obtaining high-performance device applications and monolithic integration. The disordering process in In$_{0.53}$Ga$_{0.47}$As/InP QW structures can lead to strained, disordered QWs. The model developed in this thesis for strained, disordered InGaAs/GaAs QWs is extended in this chapter to disordered InGaAs/InP single QWs, and detailed results are presented which demonstrate the effect of interdiffusion on the subband edge structure of disordered In$_{0.53}$Ga$_{0.47}$As/InP QWs.

### 7.1. Introduction

Selective area disordering of an In$_{0.53}$Ga$_{0.47}$As/InP superlattice by argon implantation has been used to modify the fundamental bandgap, and thus the refractive index, in localised areas, resulting in lateral photon confinement in optical waveguides. An impurity-free disordering process has also been used to successfully fabricate polarisation mode selective channel waveguides in an In$_{0.53}$Ga$_{0.47}$As/InP disordered...
superlattice. Selective area disordering of In$_{0.53}$Ga$_{0.47}$As/InP QWs, induced by impurity species that are introduced by ion implantation, or impurity diffusion, or by impurity-free vacancy diffusion (IFVD), can therefore provide a useful tool for bandgap engineering. Moreover, results presented here will show that disordering in In$_{0.53}$Ga$_{0.47}$As/InP QWs can, in combination with strain effects, not only modify the fundamental bandgap, but also be a source of interesting carrier confinement profiles, which could be of interest in photonic applications not directly dependent on the fundamental bandgap.

Disordering of lattice-matched AlGaAs/GaAs quantum well structures results in the interdiffusion of only group III atoms Al, Ga, as there is no As concentration gradient across the interface, while disordering of strained InGaAs/GaAs QW structures results in the interdiffusion of the group III atoms In, Ga. In comparison, the disordering of lattice-matched In$_{0.53}$Ga$_{0.47}$As/InP QW structures is more complicated since interdiffusion can occur for both group III (In, Ga) and group V (As, P) atoms, which in turn is determined by the impurity used to disorder the structure. The disordered structure may or may not be lattice-matched to InP, so that a strained-layer structure may result after interdiffusion. Another consequence of the interdiffusion processes is that either a blue-shift or a red-shift in the absorption edge is obtained depending on the impurity used to produce the interdiffusion.

7.2. Disordered InGaAs/InP Quantum Wells

The disordering of In$_{0.53}$Ga$_{0.47}$As/InP QW structures is still the subject of active investigation. The nature of the interdiffusion mechanisms in InGaAs/InP is not yet fully understood, and the role of strain in promoting or inhibiting the interdiffusion requires
further investigation. Nevertheless, the results reported generally fall into the following three categories:

(i) comparable interdiffusion rates on both group III and group V sublattices;
(ii) cation interdiffusion only;
(iii) interdiffusion on both sublattices, but with different interdiffusion rates.

Experimental results on the effects of Zn diffusion in disordered In$_{0.53}$Ga$_{0.47}$As/InP QWs have been interpreted as being due to interdiffusion of group III atoms only.$^{7,9,11,16}$ Photoluminescence (PL) measurements showed an increase in PL wavelength with disordering.$^{7,9,11,16}$ This was attributed to the interdiffusion of In and Ga, since interdiffusion of As and P would result in a lower PL wavelength.$^{7,16}$ Secondary ion mass spectroscopy (SIMS) analysis$^{7,9,10}$ and x-ray diffraction profiles$^{7,10}$ support the conclusion that in the presence of Zn diffusion the interdiffusion of the constituent atoms is confined to the cation sublattice. Transmission electron microscopy results of samples after interdiffusion revealed an absence of crystalline defects in the disordered layers within the critical thickness regime,$^{7,17}$ indicating that the disordered structure is coherently strained. Interdiffusion on both group III and group V sublattices was reported induced by sulphur diffusion,$^{7,12,18}$ by silicon diffusion,$^{7,11}$ as well as by phosphorus-ion implantation.$^{7,7}$ PL measurements show a decrease in PL wavelengths with disordering induced by S diffusion$^{7,11,18}$ and P ion implantation.$^{7,7}$ This decrease was attributed to interdiffusion on both group III and group V sublattices. Auger electron spectroscopy results indicated that comparable interdiffusion on both sublattices resulted for selected sets of conditions.$^{7,7,18}$ SIMS analysis of samples disordered using Si diffusion also indicated comparable interdiffusion on the two sublattices within a narrow range of Si concentration.$^{7,11}$ Results of impurity-free compositional disordering by repetitive rapid thermal annealing$^{7,13}$ have also been interpreted to indicate the same
extent of interdiffusion on both sublattices. Disordering by Ga implantation and subsequent annealing was observed to result in different rates of interdiffusion on the two sublattices. The results of sputtering Auger analysis for as-grown and disordered samples were interpreted as indicating that, while interdiffusion takes place on both sublattices, group III atoms interdiffuse much more than group V atoms.\(^7,8\)

Lattice-matching to InP only exists for \(\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}\) materials with \(y = 2.2(1-x)\),\(^7,19\) so that the same degree of interdiffusion on both group III and group V sublattices is required to maintain the lattice-matched condition. An interdiffusion process involving only one sublattice,\(^7,11\) or where the rate of interdiffusion on the group III and group V sublattices differs considerably,\(^7,8\) will result in a strained material system. The effects of interdiffusion on the confinement profile and subband edge structure of an undoped \(\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}\) single QW when the disordering corresponds to cases (i) and (ii) above are considered here. Details are first presented of the model used, incorporating strain and its effects, where appropriate, in order to arrive at the carrier confinement profile and subband edge structure of the disordered QW. The carrier confinement profiles and the subband edge energies and wave functions obtained when considering cation interdiffusion only are then presented and discussed. These results are contrasted with the case for identical interdiffusion on both sublattices.

7.3. Computational Considerations

7.3.1. Effects of Disordering

Consider a III-V semiconductor material \(A_xB_{1-x}C_yD_{1-y}\) where \(A,\) and \(B\) represent two group III atoms, and \(C,\) and \(D\) represent two group V atoms. After interdiffusion, let \(\bar{x},\) 1-\(\bar{x},\) \(\bar{y},\) 1-\(\bar{y}\) represent the concentration of the corresponding constituent atoms \(A,\)
B, C, and D respectively. It is assumed here that the group III and group V interdiffusion processes can be modeled by two different diffusion lengths. The interdiffusion of In and Ga atoms is characterized by a diffusion length \( L_d \), which is defined as \( L_d = (Dt)^{1/2} \), where \( D \) is the diffusion coefficient and \( t \) is the diffusion time; the interdiffusion of As and P atoms is characterized by a different diffusion length \( L_d' \). If the rates of interdiffusion on group III and group V sublattices are identical, then \( L_d = L_d' \) and the lattice-matched condition is maintained. If \( L_d' \neq L_d \), a strained QW structure results.

Consider an undoped, single In\(_x\)Ga\(_{1-x}\)As well lattice-matched to semi-infinite InP barriers. After disordering, the concentration of the interdiffused atoms across the QW structure is assumed to have an error function distribution. The constituent atom compositional profiles can, therefore, be represented as follows:

(i) in the group III sublattice, the In concentration after interdiffusion, \( x(z) \), is described by:

\[
x(z) = 1 - \frac{(1-x)}{2} \left[ \text{erf}\left(\frac{L_z + 2z}{4L_d}\right) + \text{erf}\left(\frac{L_z - 2z}{4L_d}\right) \right]
\]  

where \( L_z \) is the as-grown well width, \( z \) is the growth direction, and the QW is centred at \( z = 0 \).

(ii) in the group V sublattice, the As compositional profile after interdiffusion, \( y(z) \), is given by:

\[
y(z) = \frac{y}{2} \left[ \text{erf}\left(\frac{L_z + 2z}{4L_d'}\right) + \text{erf}\left(\frac{L_z - 2z}{4L_d'}\right) \right]
\]

where \( y = 1 \) is the As concentration of the as-grown structure.
The compositional profiles in the disordered QW structure imply that the carrier effective mass, the bulk bandgap, the strain and its effects, if present, vary continuously across the QW. Consequently, the carrier effective mass, \( m^*_{z,r}(z) \), is now z-dependent and is obtained from \( m^*_{z,r}(z) = m^*_{r}(\bar{x},\bar{y}) \), where \( m^*_{r}(\bar{x},\bar{y}) \) is the respective carrier A\( _{x} \), B\( _{1-x} \), C\( _{y} \), D\( _{1-y} \) bulk effective mass, and \( r \) denotes either the electron (C), heavy hole (V=HH), or light hole (V=LH). The unstrained (bulk) bandgap in the well, \( E_g(\bar{x},\bar{y}) \), is also a function of the compositional profile, so that the unstrained potential profile after interdiffusion, \( \Delta E_t(\bar{x},\bar{y}) \), varies across the well and is given by:

\[
\Delta E_t(\bar{x},\bar{y}) = Q_r \Delta E_g(\bar{x},\bar{y})
\]

where \( Q_r \) is the band offset and \( \Delta E_g \) is the unstrained bandgap offset.

When \( L_d' \neq L_d \) strain is introduced in the disordered structure. Consequently, the effects of strain on the bandgap, and hence on the carrier confinement profile and subband edge structure, must be considered.

### 7.3.2. Effects of Strain

If the QW layer thickness is within the critical thickness regime, the QW structure will be coherently strained after disordering,\(^7\)\(^1\) with a biaxial hydrostatic strain parallel to the interfacial plane and a uniaxial shear strain perpendicular to the interfacial plane. A compressive (tensile) hydrostatic strain causes an increase (decrease) in the bandgap energy. The shear strain disrupts the cubic symmetry of the semiconductor and lifts the degeneracy of the heavy hole (HH) and light hole (LH) band edges at the Brillouin zone centre \( \Gamma \). The heavy hole band shifts towards (away from) the conduction band and the light hole band moves away from (towards) the conduction band.\(^7\)\(^1\)\(^2\)\(^\text{1} \) In addition, the shear strain causes the LH band to couple with the spin-orbit split-off band.\(^7\)\(^2\)\(^2\)
Let $\varepsilon(\bar{x},\bar{y})$ represent the in-plane strain in the well after interdiffusion. Assuming that the growth direction $z$ is along $<001>$, then for the biaxial hydrostatic stress parallel to the interface the strain components, after interdiffusion, are given by: \[7,23\]

$$
\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon(\bar{x},\bar{y})
$$

$$
\varepsilon_{zz} = -2[\frac{C_{12}(\bar{x},\bar{y})}{C_{11}(\bar{x},\bar{y})}]\varepsilon(\bar{x},\bar{y})
$$

(4)

$$
\varepsilon_{xy} = \varepsilon_{yx} = \varepsilon_{zx} = 0
$$

where $\varepsilon(\bar{x},\bar{y})$ is defined to be negative for compressive strain, and $c_{ij}(\bar{x},\bar{y})$ are the elastic stiffness constants.

The change in the bulk bandgap due to the biaxial component of strain, $S_4(\bar{x},\bar{y})$, is given by: \[7,23\]

$$
S_4(\bar{x},\bar{y}) = -2a(\bar{x},\bar{y})[1 - \frac{C_{12}(\bar{x},\bar{y})}{C_{11}(\bar{x},\bar{y})}]\varepsilon(\bar{x},\bar{y})
$$

(5)

where $a(\bar{x},\bar{y})$ is the hydrostatic deformation potential calculated from: \[7,23\]

$$
a(\bar{x},\bar{y}) = -\frac{1}{8}[C_{11}(\bar{x},\bar{y}) + 2C_{12}(\bar{x},\bar{y})] \frac{dE_g}{dP}(\bar{x},\bar{y})
$$

(6)

where $dE_g/dP$ is the hydrostatic pressure coefficient of the lowest direct energy gap $E_g$.

The splitting energy, $S_{11}(\bar{x},\bar{y})$, between the HH and LH band edges induced by the uniaxial component of strain is given by: \[7,23\]

$$
S_{11}(\bar{x},\bar{y}) = -b(\bar{x},\bar{y})[(1 + 2C_{12}(\bar{x},\bar{y})/C_{11}(\bar{x},\bar{y})]\varepsilon(\bar{x},\bar{y})
$$

(7)

where $b(\bar{x},\bar{y})$ is the shear deformation potential. The coupling between the LH and split-off band gives rise to asymmetric heavy-hole to light-hole splitting, so that: \[7,24\]

$$
S_{11HH}(\bar{x},\bar{y}) = S_{11}(\bar{x},\bar{y})
$$

(8)

$$
S_{11LH}(\bar{x},\bar{y}) = -\frac{1}{2}[S_{11}(\bar{x},\bar{y}) + \Delta_0(\bar{x},\bar{y})] + \frac{1}{2}9[S_{11}(\bar{x},\bar{y})]^2
$$

$$
+ \{\Delta_0(\bar{x},\bar{y})\}^2 - 2S_{11}(\bar{x},\bar{y})\Delta_0(\bar{x},\bar{y})
$$

(9)

where $\Delta_0(\bar{x},\bar{y})$ is the spin-orbit splitting.
The parameters \(a, b, c_{ij}, dE_i/dP\) in eq. (4) to (7) above are assumed to obey Vegard’s law,\(^7,25\) so that their respective values depend directly on the compositional profiles across the QW.

The QW confinement potential after the disordering process, obtained by modifying the bulk post-processing potential profile with the variable strain effects, is therefore given by:

\[
U_i(z) = \Delta E_i(\bar{x},\bar{y}) - S_{\perp}(\bar{x},\bar{y}) \pm S_{\parallel}(\bar{x},\bar{y})
\]  

(10)

where \(S_{\perp}(\bar{x},\bar{y}) = Q_i S_{\perp}(\bar{x},\bar{y})\), the +ve sign represents the confined HH profile while the -ve sign represents the confined LH profile, and \(S_{\parallel}(\bar{x},\bar{y}) = 0\).

Eq. (10) represents the carrier confinement profile for the general case of a disordered InGaAs/InP QW structure, where interdiffusion on both sublattices takes place, but at different rates. It thus corresponds to case (iii) above. For the two cases of disordering considered here, eq. (10) reduces to:

for case (i):  
\[
U_i(z) = \Delta E_i(\bar{x},\bar{y})
\]  

(11)

for case (ii):  
\[
U_i(z) = \Delta E_i(\bar{x},1) - S_{\perp}(\bar{x},1) \pm S_{\parallel}(\bar{x},1)
\]  

(12)

7.3.3. Subband Edge Calculation

The electron and hole subband structure at \(\Gamma\) can be determined by considering the appropriate Schrödinger equation from the Ben Daniel-Duke model,\(^7,26\) using the envelope function scheme\(^7,27\) with an effective mass approximation. The one-electron Schrödinger equation for the disordered QW can be expressed as:

\[
-\frac{\hbar^2}{2m_{\ell}(z)} \frac{d}{dz} \left[ \frac{1}{m_{\ell}^*(z)} \frac{d\chi_n(z)}{dz} \right] + U_i(z)\chi_n(z) = E_n\chi_n(z)
\]  

(13)
where the growth direction $z$ is the confinement axis, $\chi_\ell(z)$ is the envelope wave function, $E_\ell$ is the quantized energy level with the subband energy zero at the bottom of the QW, and $\ell = p$ or $q$ refers to the quantized subband energy levels for the electron and holes, respectively. This equation is solved numerically to obtain the quantized energy levels $(E_{cp}, E_{vq})$, and the envelope wave functions $(\chi_{cp}, \chi_{vq})$. Hence the interband transitions energy can be determined, as well as the overlap integral $<\chi_{cp}|\chi_{vq}>$ between the $p$th conduction subband and the $q$th valence subband envelope functions.

7.4. Results and Discussion

A 6 nm thick undoped In$_{0.35}$Ga$_{0.65}$As single QW layer sandwiched between thick InP barriers is considered and results obtained for various stages of disordered. The as-grown structure is lattice-matched and the effects of disordering on the QW structure are considered here for group III sublattice interdiffusion only, and for identical interdiffusion for both group III and group V sublattices. The parameters for the disordered structure were determined by interpolating between the binary parameters detailed in Table 7.1. The generalized parameter $T$ for the quaternary material $A_{x}B_{1-x}C_{y}D_{1-y}$ constructed from the four binary compounds AC, AD, BC, and BD can be derived from the four binary parameters using the interpolation scheme:$^{7,25}$

$$T(x,y) = (1-x)yT_{BC} + xyT_{AC} + x(1-y)T_{AD} + (1-x)(1-y)T_{BD}$$ (16)

The room temperature bulk bandgap compositional dependence, in eV, was calculated using:$^{7,28}$

$$E_g(x,y) = 1.35 - 1.17y + 0.668(1-x) - 0.069(1-x)y + 0.18y^2$$
$$+ 0.03(1-x)y^2 + 0.758(1-x)^2 - 0.322(1-x)y$$ (17)

while the spin-orbit splitting, in eV, was obtained from:$^{7,25}$

$$\Delta_s(x,y) = 0.34(1-x)y + 0.43xy + 0.10(1-x)(1-y) + 0.10x(1-y)$$ (18)
Table 7.1.

Material parameters of GaAs, InAs, GaP, InP used in the numerical calculations. $a_0$ is the lattice constant, $m_0$ is the electron mass in free space. Values are taken from Ref. 7.25 unless otherwise indicated.

<table>
<thead>
<tr>
<th></th>
<th>GaAs</th>
<th>InAs</th>
<th>GaP</th>
<th>InP</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>5.6533</td>
<td>6.0584</td>
<td>5.4512</td>
<td>5.8688</td>
<td>Å</td>
</tr>
<tr>
<td>$c_{11}$</td>
<td>11.88</td>
<td>8.329</td>
<td>14.12</td>
<td>10.22</td>
<td>$10^{11}$ dyn/cm$^2$</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>5.38</td>
<td>4.526</td>
<td>6.253</td>
<td>5.76</td>
<td>$10^{11}$ dyn/cm$^2$</td>
</tr>
<tr>
<td>$dE_g/dP$</td>
<td>11.5</td>
<td>10.0</td>
<td>11.0</td>
<td>8.5</td>
<td>$10^{6}$ eV/bar</td>
</tr>
<tr>
<td>$b$</td>
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<td>-1.8</td>
<td>-1.5</td>
<td>-2.0</td>
<td>eV</td>
</tr>
<tr>
<td>$m^*_c$</td>
<td>0.067$^a$</td>
<td>0.023</td>
<td>0.17</td>
<td>0.08</td>
<td>$m_0$</td>
</tr>
<tr>
<td>$m^*_{\text{III}}$</td>
<td>0.34$^a$</td>
<td>0.60</td>
<td>0.79</td>
<td>0.85</td>
<td>$m_0$</td>
</tr>
<tr>
<td>$m^*_{\text{LH}}$</td>
<td>0.087$^b$</td>
<td>0.027</td>
<td>0.14</td>
<td>0.089</td>
<td>$m_0$</td>
</tr>
</tbody>
</table>

$^a$ Reference 7.30.

$^b$ Reference 7.31.
Different experimental techniques have resulted in various values for the conduction band offset $Q_c$ of In$_{0.53}$Ga$_{0.47}$As/InP heterostructures$^{7,29}$; $Q_c = 60\%$ was used here.

### 7.4.1. Group III Interdiffusion Only

The constituent atom compositional profiles after interdiffusion of the group III atoms only are shown in Fig. 7.1(a). Ga atoms diffuse into the InP barrier while In atoms diffuse into the QW, forming an InGaP/InGaAs interface. After interdiffusion, the Ga and In concentration profiles are described by the error function distribution, while the As and P concentration profiles do not change, thereby maintaining an abrupt change at the interface. Since the InP lattice constant is always larger than that of InGaP, a tensile strain arises in the barrier near the interface, while the InGaAs well becomes compressively strained due to the increased In content. Consequently, the disordering process results in a strained QW structure, with the strain profile across the structure as shown in Fig. 7.1(b). This strain profile affects the shape and separation of the conduction and valence bands, and the HH and LH potential wells no longer coincide. The confinement profile of the disordered structure remains abrupt with a width equal to that of the as-grown QW, as shown in Fig. 7.1(c). This is due to the bandgap change from InGaP to InGaAs at the interface and is in contrast to the graded confinement profiles that result when comparable interdiffusion on both sublattices occurs in In$_{0.53}$Ga$_{0.47}$As/InP QW structures (see below), and in the case of the more extensively studied AlGaAs/GaAs$^{7,20}$ and of InGaAs/GaAs$^{7,32}$ disordered QWs.

The confinement profile shown in Fig. 7.1(c) presents interesting features at the top of the well, near the continuum, and at the bottom of the well. A potential build-up occurs in the barrier at the interface because the bulk bandgap of InGaP is greater than
Fig. 7.1. Profiles of (a) composition (b) in-plane strain, (c) electron(C), HH, and LH confinement potential for $L_z = 6$ nm, $L_d = 1$ nm, $Q_c = 60\%$, with well centre at $z = 0$, considering cation interdiffusion only.
that of InP. However, this potential build-up is significantly modified by the effects of the tensile strain in the barrier near the interface, and can even be reversed by strain, as will be shown below for the LH well. Inside the well, the In content at the well centre is less than that at the interface so that the bulk (unstrained) bandgap at the centre is larger than that at the interface. The compressive strain is much smaller at the well centre so that the strain effects on the bandgap are much more pronounced at the interface. The combination of the bulk bandgap and the compressive strain effects on this bandgap results in the potential at the well centre being higher than at the interface, and this gives rise to two "miniwells". The strain dependent splitting of the HH and LH subbands in opposite directions causes the HH subband to have the deepest miniwells and the LH subband to ultimately result in an almost flat-bottomed well. The results indicate that in the case of the HH confinement profile, the subband ground state can be supported at energy levels that lie within the miniwells.

Details of the effects of strain on the carrier confinement profile, for \( L_z = 6 \text{ nm} \) and \( L_d = 1 \text{ nm} \), are presented in Fig. 7.2, which shows the effect of the hydrostatic and shear components of strain on the unstrained bandgap, and the final confinement profile. Since only the hydrostatic component of strain modifies the electron confinement profile, the final confinement profile in this case coincides with the profile as modified by the effects of the hydrostatic component of strain. This is shown in Fig. 7.2(a) where it can be seen that the compressive strain in the InGaAs well reduces the depth of the miniwells while the tensile strain in the barrier near the interface reduces the potential build-up at the top of the well. Thus strain reduces the depth of the electron confinement profile. The hydrostatic component of the compressive strain in the InGaAs well again reduces the depth of the miniwells for both the HH and LH cases, as shown in Fig. 7.2(b), and 7.2(c), respectively, but the shear component of the compressive strain results in opposite
Fig. 7.2. Effects of strain and disordering on (a) electron, (b) HH and (c) LH confinement profiles in a disordered In$_{0.55}$Ga$_{0.47}$As/InP single QW, considering cation interdiffusion only. The dashed lines represent the unstrained bandgap after disordering, and the dot-dash lines show how the unstrained bandgap is modified by the effects of hydrostatic strain. The solid lines represent the final carrier confinement profile. The potential is taken to be zero at the well centre, z = 0, for the unstrained bandgap, in each case. QW details: $L_z = 6$ nm, $L_d = 1$ nm.
shifts of the HH and LH confinement profiles; the HH miniwells now become deeper, while the LH miniwells disappear. The tensile strain in the barrier near the interface also modifies the confinement profile. The hydrostatic component reduces the height of the potential build-up for both the HH and LH confinement profiles. The shear component of the tensile strain again produces opposite effects on the HH and LH confinement profiles, so that the potential build-up height increases again in the case of the HH case, while in the LH case this potential build-up disappears and, depending on the extent of the interdiffusion, may actually be reversed, see Fig. 7.2(c). The overall result is that the strain produced in the disordered InGaAs/InP structure increases the depth of the HH confinement profile whilst it decreases the LH confinement profile depth.

The splitting of the HH and LH confinement profiles at \( \Gamma \) caused by the shear component of the compressive strain in the InGaAs well and by the shear component of the tensile strain in the barrier near the interface is shown in Fig. 7.3. As already noted, this splitting strongly modifies the HH and LH confinement profiles and a significant difference in the depth of the HH and LH wells results. For the case considered here, the HH confinement profile depth at the interface is about 440 meV, while the LH confinement profile depth at the interface is about 200 meV.

The electron(C) and HH subband edge structure for the numerical case \( L_x = 6 \text{ nm}, L_d = 1 \text{ nm}, \text{ and } Q_c = 60\% \), are shown in Fig. 7.4. Five subband states result in the HH well with the HH ground state lying near the top of the miniwells. The square of the envelope wave function of the first HH subband state, \( |\psi_{hh1}|^2 \), is shown in Fig. 7.5(a), and indicates that the HH1 carrier couples between the miniwells. The HH5 energy level is at the top of the well where the barrier is sufficiently thin (~0.5 nm) for the carrier to tunnel out of the well even in the absence of an applied electric field, and this state can no longer be considered bound. The conduction well, on the other hand, supports
Fig. 7.3. The strain induced HH-LH band edge splitting in the well, and in the barrier close to the interface, considering group III interdiffusion only, for $L_z = 6$ nm and $L_d = 1$ nm. The dashed lines show the unstrained bandgap after interdiffusion, the dot-dash lines show how this bandgap is modified by the hydrostatic strain, and the solid lines represent the final confinement profile.
Fig. 7.4. The confinement profile, and the confined subband states for (a) electron, (b) HH, of a disordered \( \text{In}_{0.55}\text{Ga}_{0.45}\text{As}/\text{InP} \) single QW, considering cation interdiffusion only, for \( L_z = 6 \) nm, \( L_d = 1 \) nm, and \( Q_c = 60\% \). The potential zero is taken at the well centre.
Fig. 7.5. $|\chi|^2$ for (a) HH1, and (b) C2 subband states for the disordered In$_{0.53}$Ga$_{0.47}$As/InP QW, considering group III interdiffusion only.
two confined subbands. By careful optimization of the disordering process a quasi-bound first excited state at an energy level close to the continuum can be obtained in the conduction well. Because of the presence of the potential build-up caused by the tensile strain in the barrier close to the interface, the envelope wave function of the first excited state would still be fairly well confined, as shown in Fig. 7.5(b). With the application of an external electric field, the electron in this first excited state is expected to tunnel out of the conduction well, which may be of interest for device applications.

The variation of strain at a point on either side of, and close to, the interface and at the well centre, as the interdiffusion proceeds, is shown in Fig. 7.6(a). In the initial stages of interdiffusion ($L_d = 1$ nm), the Ga atoms diffuse into the InP barrier so that the Ga concentration at a point in the well close to the interface drops sharply while at a point in the barrier close to the interface it rises sharply, and the changes at the well centre are insignificant. Subsequent interdiffusion, however, leads to a rapid reduction of the Ga concentration at the well centre as the Ga atoms diffuse deeper into the barrier and tend towards a uniform distribution across the structure. This explains the in-plane strain curves of Fig. 7.6(a) where it can be seen that the difference between the strain at the well centre and at a point in the well close to the interface is greatest for $L_d = 1$ nm. This strain difference within the well affects the depth of the miniwells. For the well width considered here, the HH miniwells have a maximum depth of about 90 meV, around $L_d = 1$ nm. For $L_d > 6$ nm and higher, the strain profile across the well is almost linear, reflecting a more uniform Ga concentration across the well, while for large $L_d$ the miniwells no longer exist. At the interface a lattice mismatch of $\sim 3.1\%$ exists which is almost independent of the extent of the interdiffusion, and is in agreement with reported experimental results.7,11

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Fig. 7.6. Cation interdiffusion only. (a) Strain variation with $L_d$ at three points in the QW structure: (i) in the barrier, close to the interface, (ii) at the well centre, and (iii) in the well, close to the interface; (b) ground state transition energy variation with $L_d$. 
The variation of C1-HH1 and C1-LH1 transition energy with interdiffusion is shown in Fig. 7.6(b). The QW bandgap energy is the C1-HH1 transition, reflecting the compressive nature of the strain induced in the QW by the disordering process. The HH1 state occurs in the miniwells for small values of \( L_d \). As the interdiffusion proceeds the bandgap energy decreases, corresponding to a shift to longer wavelengths, as shown by experimental results for Zn induced disordering.\(^7,9,11\) The shift of the band edge wavelength to longer wavelengths with disordering contrasts with the experimental results for disordered AlGaAs/GaAs\(^^{7,20}\) and InGaAs/GaAs\(^\text{7,33}\) and for InGaAs/InP with a comparable extent of interdiffusion for the two sublattices, where the band edge wavelength shifts to shorter wavelengths, as discussed below. For the interdiffusion length range in Fig. 7.6(b) the shift in bandgap energy corresponds to a shift in band edge wavelength from about 1.4 \( \mu \text{m} \) to about 1.9 \( \mu \text{m} \). Another contrasting effect is the difference between the C1-HH1 and C1-LH1 transition energy. It can be seen from Fig. 7.6(b) that disordering under these conditions leads to an increased separation between the C1-HH1 and C1-LH1 transition energy, while in disordered InGaAs/GaAs QW structures this separation decreases.\(^7,34\)

**7.4.2. Identical Interdiffusion Rate For Group III and Group V Sublattices**

When the rates of interdiffusion for the two sublattices are comparable, the structure remains lattice-matched. The error function distribution is again used to describe the constituent atom compositional profiles after interdiffusion, which are shown in Fig. 7.7(a). The \( \text{In}_{0.53}\text{Ga}_{0.47}\text{As} \) well now changes to \( \text{InGaAsP} \) with a larger energy bandgap which is lattice-matched to the InP semi-infinite barrier. The results of Fig. 7.7 show that after interdiffusion, the confinement profiles are no longer abrupt and the HH and LH profiles still coincide since no strain is present. The C1-HH1, C1-LH1 transition
Fig. 7.7. Profiles of (a) composition, and (b) electron(C), HH, and LH confinement potential for $L_x = 6$ nm, $L_d = 1$ nm, and $Q_c = 60\%$, considering identical interdiffusion rates on group III and group V sublattices; (c) ground state transition energy variation with $L_d$. 

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energies increase as disordering increases, which results in a bandgap shift to shorter wavelengths, as reported for disordered InGaAs/InP using for example S diffusion\(^{7,12}\) as well as for disordered AlGaAs/GaAs\(^{7,20}\) where the interdiffusion process is much better understood. The change in the C1-HH1 transition energy in going from \(L_d = 0\) to 10 nm corresponds to a shift to shorter wavelengths of about 400 nm, from about 1.4 \(\mu\)m to about 1.0 \(\mu\)m, which is much larger than that for InGaAs/GaAs\(^{7,34}\) and is a direct result of the compositional changes brought about by the disordering process. The C1-HH1 and C1-LH1 transition energies converge as \(L_d\) increases so that in the disordered InGaAs/InP structure the separation between the two transition energies almost reduces to zero. Since the disordered structure remains lattice-matched, the HH and LH confinement profiles still coincide, and the difference between the two transition energies is simply the result of the different quantization effects for the HH and LH due to their different effective masses. As interdiffusion proceeds, an effectively wider well results\(^{7,32}\) and the difference in the quantization effects for the HH and LH therefore decreases. This is in contrast to the results obtained above for the case of cation interdiffusion in InGaAs/InP where the presence of strain results in increased separation between the C1-HH1 and C1-LH1 transition energies.

7.5. Summary

The disordering of lattice-matched InGaAs/InP single QWs has been studied by using an error function to model the compositional profile after interdiffusion. Cation interdiffusion results in the formation of an InGaP/InGaAs abrupt interface. During the early stages of interdiffusion a large strain build-up across the well is produced. The strain and its effects on the unstrained bandgap profile of the disordered structure produces a distinctive carrier confinement profile which remains abrupt even after
significant interdiffusion, with a well width equal to that of the as-grown QW, which is in contrast to other material systems such as AlGaAs/GaAs and InGaAs/GaAs. The effects of strain combined with the unstrained bandgap profile results in a potential build-up in the barrier near the interface, at the top of the well, while it gives rise to two miniwells at the bottom of the wells. The HH and LH band edge splitting results in two distinct HH and LH confinement profiles with different depths. The subband edge structure of the disordered QWs has been presented, showing that the HH well can support the ground state within these miniwells. Both the conduction and HH wells can support states at the top of the well where, as a result of the potential build-up, the barrier is sufficiently thin for the carriers to tunnel out even in the absence of an electric field. The ground state (C1-HH1) transition shifts to longer wavelengths, and an increased separation between the C1-HH1 and C1-LH1 transition energy results due to strain. By optimizing the disordering process, the potential build-up at the top of the well can be of interest in applications dependent on intersubband transitions and on carrier tunnelling. When comparable interdiffusion on both sublattices takes place, the structure remains lattice-matched, and the confinement profile changes to a graded profile. The C1-HH1 transition energy shifts to shorter wavelengths, while there is a decrease in the separation between the C1-HH1 and C1-LH1 transition energy. This is similar to disordered AlGaAs/GaAs and InGaAs/GaAs QW structures.

The model presented here accounts for reported experimental results for the disordering of In_{0.95}Ge_{0.05}As/InP QWs both in the case of cation interdiffusion only, and for identical interdiffusion on both sublattices. At the same time, by taking strain effects into consideration, it reveals interesting features in the carrier confinement profiles and subband edge structure that arise in the case of cation interdiffusion, which may be of use in both electronic and optical device applications.
The results presented provide an example of the potential of using QW disordering as a process which is more than a simple bandgap engineering tool. In the case of disordered In$_{0.53}$Ga$_{0.47}$As/InP QWs, it has been shown that, in combination with strain effects, which themselves are a result of the disordering process, interesting carrier confinement profiles can result, which could lead to applications not directly related to the change in the fundamental bandgap brought about by disordering.
7.6. References


Chapter 7


CONCLUSIONS AND FURTHER WORK

8.1. Conclusions

In this thesis, the effects of disordering on coherently strained InGaAs/GaAs single QWs and on In_{0.53}Ga_{0.47}As/InP single QWs have been modelled with a view to obtaining an insight into the use of strain and QW disordering as a tool for bandgap engineering with potential applications in quantum well photonic devices, such as photodetectors, waveguides, and modulators. The carrier confinement profiles, subband edge structure, and optical properties of undoped, strained, disordered InGaAs/GaAs single QWs have been determined by taking into consideration the combined effects of compressive strain and constituent atoms interdiffusion. An error function distribution is assumed for the compositional profile after interdiffusion.

The results presented in this work show that the optical properties of strained QWs, such as the absorption coefficient and the refractive index, can be usefully varied in a controlled manner by disordering. The results demonstrate that disordering of strained InGaAs/GaAs QWs can potentially be an attractive proposition for a number of purposes, such as designing a photonic application for a specific wavelength around 1 \( \mu \text{m} \), optimising the device performance of electroabsorption modulators, and improving the possibility of monolithic integration. Furthermore, calculations carried out for InGaAs/GaAs QWs with different In content illustrate the flexibility offered by disordered, strained QW structures in exploiting this potential, as a result of the absence of the lattice-matching constraint. In the course of the theoretical investigations it has
also become apparent that strain and disordering can also be a source of distinctive carrier confinement profiles which do not arise in disordered, lattice-matched QW structures, and which could be of interest for photonic applications.

In considering the results obtained here, it is important to note that certain assumptions were made, including parabolic carrier effective masses and negligible valence band mixing effects, and that there is still considerable discussion on the values of certain parameters used in the numerical calculations. In InGaAs/GaAs QWs there is uncertainty as to the value of the band offset ratio and on whether the electrons and light holes are spatially separated. The value used here for the band offset ratio, and the significant strain-induced HH-LH band edge splitting result in a very shallow light hole confinement profile in the compressively strained InGaAs layer, and the results show that the effects of the light hole transitions on the optical properties near the fundamental absorption edge are quite small, even for the disordered InGaAs/GaAs structure.

The fundamental absorption edge is an important parameter in photonic devices such as photodetectors and modulators, and its dependence on strain and disordering is of considerable interest. In strained QW structures the depth of the carrier confinement profiles is significantly altered by the strain. In the case of InGaAs/GaAs the results show that, starting with a valence band offset ratio of 30%, the compressive strain in the InGaAs layer can lead to a heavy hole band offset ratio of almost 50%. Thus strain is an additional parameter offering the possibility of altering the ground state transition energy in an as-grown QW structure, providing an extra degree of freedom in tailoring the fundamental absorption edge. Disordering of strained QW structures adds to this flexibility by providing the possibility of continuous bandgap modification, resulting in a continuous shift of the fundamental absorption edge to shorter wavelengths. Of course, disordering of lattice-matched QWs also results in continuous bandgap modification, but
the ground state transition energy for different as-grown lattice-matched QW structures is practically fixed (except for quantum size effects) for a particular material system. In strained QW structures, it is possible to choose the composition of the as-grown well layer because of the lifting of the lattice-matching constraint, so that different values of the ground state transition energy can be obtained for different as-grown QW structures. This is a significant advantage over lattice-matched QW structures. Furthermore, because of the presence of strain, the amount of absorption edge shift in the disordered structures is enhanced.

The absorption coefficient spectra for disordered, strained InGaAs/GaAs single QWs for light propagating parallel to the QW layer and for normal incidence, exhibit well defined exciton peaks which shift to shorter wavelengths with interdiffusion. The results show that the absorption edge in disordered InGaAs/GaAs can be tailored to desired wavelengths around 1 μm. This ability to tune the absorption edge demonstrates a fundamental use of QW disordering, i.e. designing for a photonic application, such as a demultiplexer, at a specific wavelength. Furthermore, careful control of the disordering process can lead to selected areas in a single chip having different absorption edges. This is a primary requirement in the monolithic integration of devices performing different functions. Significant separation between the fundamental absorption edge for TE and TM polarisation results due to the presence of the compressive strain in the InGaAs layer. This is in contrast with lattice-matched QW structures, where the polarisation sensitivity, which is a function only of the different hole effective masses, is significantly less. This polarisation sensitivity decreases with increasing interdiffusion since the strain in the disordered structure decreases. These results may be useful for polarisation sensitive applications.
The changes in the absorption coefficient spectra caused by disordering of InGaAs/GaAs QWs also lead to changes in the refractive index of the disordered, strained QW structure. For wavelengths > 1 μm the refractive index decreases as the extent of disordering increases, resulting in a positive refractive index step with respect to the as-grown, or the less disordered, structures. This lateral refractive index step is larger when the confining regions are more extensively disordered. Results also show that the positive refractive index step increases with decreasing well widths, or with increasing In content. Partly as a result of strain in InGaAs/GaAs QWs the refractive index step is more sensitive to the In content than to the QW width. These results show that selective area QW disordering is a potentially important process in providing strong lateral confinement of photons in strained QW structures, which is indispensable for the monolithic integration of semiconductor lasers with waveguides and modulators.

The potential of using disordering to achieve improved performance of InGaAs/GaAs QW electroabsorption modulators is also supported by the results presented here. The results obtained for disordered InGaAs/GaAs single QWs show that for a sufficiently large value of $L_d$ the exciton Stark shift in the disordered QW is greater than in the as-grown QW. Calculations also show that the change in electroabsorption around the fundamental absorption edge is larger in the disordered QW than in the as-grown QW for the same applied field. This implies that disordering of InGaAs/GaAs QWs could be used to achieve an improved on/off ratio or reduced device length in waveguide modulators for wavelengths around 1 μm. This makes the disordered structure attractive for the integration of small size devices.

The effects of the disordering process in In$_{0.33}$Ga$_{0.67}$As/InP QW structures, which can lead to strained, disordered QWs has also been investigated. In contrast to both strained InGaAs/GaAs and lattice-matched AlGaAs/GaAs disordered QWs, cation
interdiffusion only in In$_{0.53}$Ga$_{0.47}$As/InP leads to a shift of the fundamental absorption edge to longer wavelengths. The results presented show that disordering in In$_{0.53}$Ga$_{0.47}$As/InP QWs can, in combination with strain effects, not only modify the fundamental bandgap, but also be the source of interesting confinement profiles, which are quite distinct from those of disordered InGaAs/GaAs and AlGaAs/GaAs QWs, and which could be useful in photonic applications. An abrupt confinement profile is maintained after interdiffusion, miniwells arise at the bottom of the potential wells and a potential build-up occurs in the barrier near the interface at the top of the wells. The heavy hole well can support the ground state within the miniwells, while the potential build-up can lead to quasi-bound states. These results provide an example of the potential of using QW disordering as a process which, in combination with strain, is more than a bandgap engineering tool.

In conclusion, the results presented in this thesis show that disordering and strain in InGaAs based QW structures can provide a useful tool for bandgap engineering with particular reference to photonic applications at wavelengths $\geq 1 \mu m$, and that in certain cases characteristics result which are not attainable in lattice-matched, disordered QW structures. Optical properties have been modelled, demonstrating the possibility of tuning the fundamental absorption edge of InGaAs/GaAs QW structures around $1 \mu m$, providing a lateral refractive index step for the confinement of photons in as-grown, or less disordered regions, and showing the potential of improving device performance in electroabsorption modulators. These results indicate the potential use of disordering of strained QW structures also in the context of monolithic integration. The results obtained when extending the model to disordered In$_{0.53}$Ga$_{0.47}$As/InP QWs also show that QW disordering, in combination with strain, can not only be used as a bandgap engineering tool, but can also be the source of novel confinement profiles that could prove useful for photonic applications not directly dependent on the fundamental bandgap.
8.2. Further Work

The theoretical investigation carried out in this thesis into the carrier confinement profiles and optical properties of strained, disordered single QW structures can be extended in several ways. Different strained material systems which are being investigated experimentally for photonic applications can be studied, such as InGaAs/AlGaAs, and InGaAs/InP (both compressively strained and tensile strained InGaAs layers). For tensile strained QW structures, valence band mixing effects would need to be considered in more detail. Recent experimental investigation of the disordering of GaInP/GaAs QWs indicated that a strained QW structure could result after interdiffusion, so that the model can be applied to study the carrier confinement profiles of disordered GaInP/GaAs QWs. The model can be extended to investigate strained QW structures grown on compositionally-graded buffer layers, where both well and barrier layers are strained. Thus for InGaAs/GaAs structures, the compressive strain in the InGaAs layer and the tensile strain in the GaAs barrier would need to be taken into consideration. These structures are the object of recent experimental investigation, since improvements in epitaxial growth have enabled good quality strained-layer structures to be fabricated on compositionally-graded buffer layers.

The ideal single quantum well considered here needs extension to multiple quantum well (MQW) structures, enabling the characteristics of realistic QW structures for waveguide and modulator applications to be more accurately investigated. The compositional profile after interdiffusion for the MQW should be different from that considered here for the single QW since the barrier would now be a source of limited extent, similar to the well, except for the barriers acting as cladding layers, which would still provide an infinite source. The strain profile in the disordered MQW structure would consequently also be different from that in the single QW model.
These extensions of the theoretical studies and other effects would enable a wider investigation into the possibility of combining strain and disordering for bandgap engineering, and as a source of distinctive confinement profiles, aimed at improved photonic device performance, as well as for the purposes of furthering the realisation of monolithic integration. At the same time experimental verification of the theoretical results presented here should also be carried out. For instance, the effects of different disordering process temperatures and times on the fundamental bandgap and subband structure of single QWs can be investigated using techniques such as room temperature photoreflectance and low temperature photoluminescence.
8.3. References


