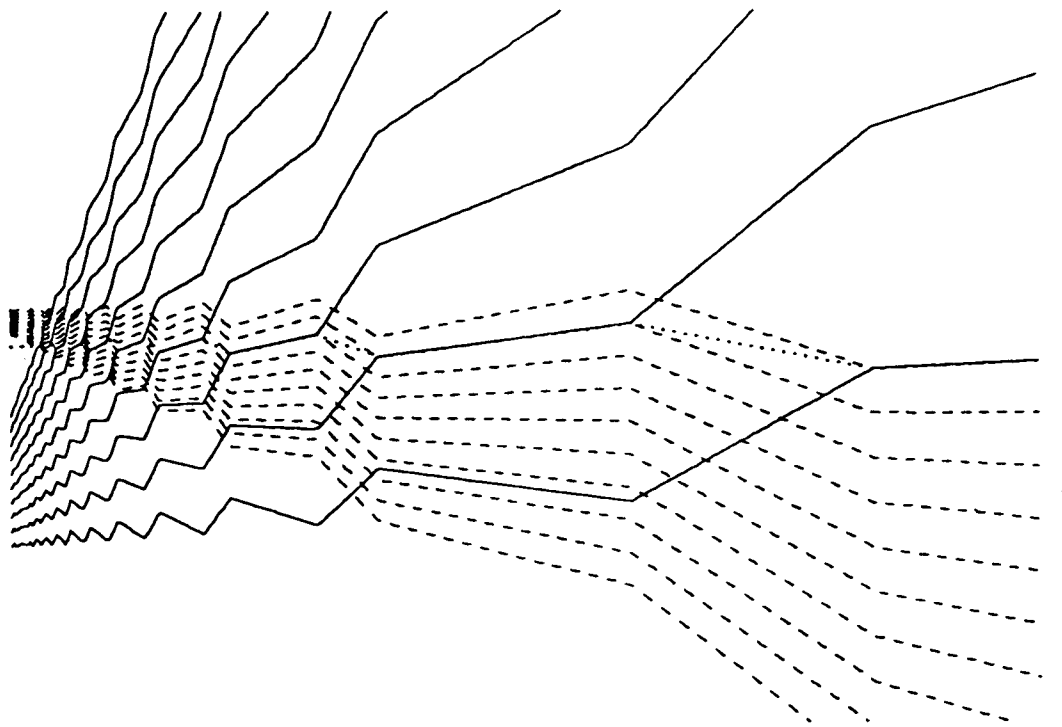
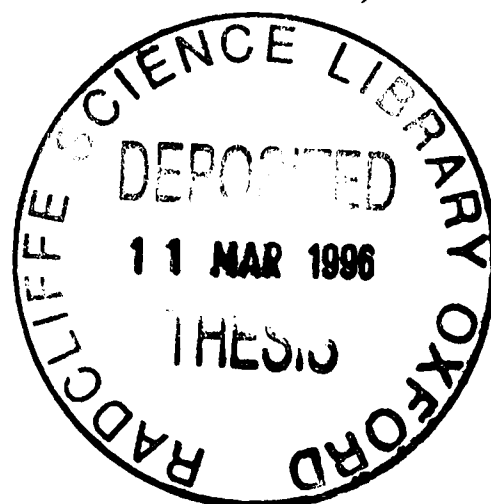


Magneto-Optics of InAs/GaSb Heterostructures

Thomas Alexander Vaughan



A thesis submitted for the degree of Doctor of Philosophy
Brasenose College, Oxford
Michaelmas Term, 1995



Magneto-optics of InAs/GaSb Heterostructures

Thomas Alexander Vaughan

A thesis submitted for the degree of Doctor of Philosophy
Brasenose College, Oxford
Michaelmas Term, 1995

Abstract

The optical properties of InAs/GaSb heterostructures under applied magnetic fields are studied in experimental and theoretical detail. The InAs/GaSb system is a type-II “crossed-gap” system, where the valence band edge of GaSb lies higher in energy than the conduction band edge of InAs. This leads to a region of energy above the InAs conduction band where conduction and hole states mix. Thin-layer superlattices remain semiconducting due to confinement effects, but thick-layer superlattices experience charge transfer which leads to intrinsic carrier densities approaching 10^{12} cm^{-2} per layer.

Existing multi-band modeling techniques based on the $k \cdot p$ formalism are discussed, and a method of solving superlattice band structure (the “momentum-matrix” technique) is presented. The quantizing effects of the superlattice layers and applied magnetic fields are investigated, and the selection rules for optical transitions are derived.

Standard cyclotron resonance (CR) is used to study effective masses in InAs/GaSb structures. The heavy hole mass is found to be strongly orientation-dependent, with a mass in the [111] orientation reduced 25% from the [001] mass. The electron mass is found to be roughly isotropic with respect to growth orientation, but shows variation with the InAs width due to quantum confinement effects. CR of InAs/GaSb heterojunctions display hitherto unexplained oscillations in linewidth, intensity, and effective mass. A model is proposed which explains the oscillations, based on the intrinsic nature of the InAs/GaSb system.

CR is performed on an InAs/GaSb heterojunction using a free-electron laser, where due to the high intensities (on the order of MW/cm^2) the absorption process saturates. This saturation allows for a determination of non-radiative relaxation lifetimes, and through the energy dependence of these lifetimes the magnetophonon effect is observed, allowing a direct measurement of LO-phonon-assisted energy relaxation rates.

Coupling is introduced into the standard CR experiment, either by tilting the sample with respect to the magnetic field, or by applying a metal grating to the surface. These coupled CR experiments have striking qualitative results which allow for determination of subband separation energies and coupling matrix elements.

Photoconductivity experiments are performed on thin-layer (semiconducting) superlattices, showing optical response at far-infrared wavelengths (5-20 μm). The results are compared with $k \cdot p$ calculations. One sample is processed for vertical transport, in which conduction occurs perpendicular to the superlattice layers. Strong optical response from this sample indicates the viability of InAs/GaSb-based far-infrared detectors.

The momentum-matrix technique is used to predict optimum parameters for semiconducting superlattices with band gaps in the far-infrared. Semimetallic structures are studied via a multi-band self-consistent model, with results corroborating with and extending previous work. Intrinsic structures under applied magnetic field are modeled theoretically for the first time.

Acknowledgements

I would like to thank all who have assisted in the preparation of this thesis, in particular:

Prof. P. G. H. Sandars, Prof. R. A. Cowley and Dr. J. M. Baker for extending to me the facilities of the Clarendon Laboratory.

My supervisor, Dr. Robin Nicholas, for his enthusiasm and many experimental and theoretical insights, and his tolerance with Washington wine makers.

Dr. P. J. Walker and Dr. N. J. Mason for growing the samples that made this research possible, and for their useful if somewhat pessimistic appraisal of each sample's potential.

My research colleagues: M'hamed Lakrimi, 2nd in command of the Nicholas Empire, for teaching me everything I know about experimental techniques, and a fair amount of football as well; Glen "Cryosoft" Summers, for extremely useful computing advice and in-depth analysis of Nicholas group mountaineering expeditions; Joe Michels, for practical advice on how to deal with sense of humor failures, and for a demonstration of how to run up the Zugspitze; Dave Symons, amazing rollerblader and master of transport, for a spirited exposition on how $k \cdot p$ matrices could be applied to billiards; Matt Daly, whose skill at football is matched only by his competitive spirit, for unusual adjectives and a refined appreciation for Guinness; Dave "Tourette's" Kinder, for teaching me nothing whatsoever about sarcasm, and for his unwavering high opinion of all MicroSoft™ products; Henry Chen, for programming $k \cdot p$ almost as fast as he drives, for many useful discussions; Maarten van der Burgt, famous Belgian and fellow *Kuifje* aficionado; John Dykema, the California surfer dude with a knack for infrared physics; Richard Warburton, Nicholas group liaison with irritable German hotel keepers, for introducing me to my first 8x8; Yifang Chen, who seems to have a camera at all the wrong times; and also Alice Wong, Rob Martin, Andrew Priest, Karen Dalton, Chin-Chi Chang, Javed Rehman, Sungwon Khym, and Andrew Poulter.

The technical staff at the laboratory, especially Dennis Rawlings for fixing the inserts every time I broke them, and George Matthews for considerable help in the workshop and interesting conversations at tea.

My fellow data junkies and coffee-bean activists at FELIX, Casper Langerak and Ben Mordin.

My friends and associates at WPAFB and Wright State University in Dayton, Ohio, who introduced me to semiconductor physics, particularly my research supervisor there Dr. Frank Szmulowicz, without whose influence I'd probably be flipping burgers somewhere.

The National Science Foundation, Overseas Research Student awards, Brasenose College, the Institute of Physics, and the Clarendon Laboratory for financial support.

This thesis is dedicated to my parents for their love and support throughout my education.

Table of Contents

Chapter 1: Introduction	1
1.1 SCOPE OF THE THESIS	2
1.2 OVERVIEW	2
1.3 BULK MATERIALS.....	3
1.4 HETEROSTRUCTURES	4
1.5 THE INAs/GaSb SYSTEM.....	6
1.6 GROWTH TECHNIQUES.....	8
1.7 MAGNETIC FIELD	9
1.8 UNITS	10
1.9 REFERENCES	10
Chapter 2: $k \cdot p$ Theory and the Envelope Function Approximation	12
2.1 BULK LATTICES: $k \cdot p$ THEORY.....	13
2.1.1 Framework of $k \cdot p$ Theory.....	13
2.1.2 Solving for Bulk Eigenstates.....	15
2.1.3 Expanding around a Special Point in the Brillouin Zone.....	15
2.1.4 Constructing Bulk Hamiltonians.....	16
2.2 HETEROSTRUCTURES: THE ENVELOPE FUNCTION APPROXIMATION.....	21
2.2.1 Framework of the Envelope Function Approximation.....	21
2.2.2 The Transfer-Matrix Technique	28
2.2.3 The “Momentum-Matrix” Technique	34
2.2.4 Choice of a Basis Set	38
2.3 APPLICATION OF MAGNETIC FIELD	39
2.4 OBSERVABLES: TRANSITIONS AND SELECTION RULES	41
2.4.1 Zero Magnetic Field	42
2.4.2 Applied Magnetic Field	43
2.4.3 Type-I versus Type-II Selection Rules	43
2.4.4 Influences of Far Bands.....	44
2.5 FINAL NOTE	45
2.6 REFERENCES	45

Chapter 3: Cyclotron Resonance 48

3.1 INTRODUCTION 49

3.2 EXPERIMENTAL SETUP 49

3.3 THEORY 50

3.4 EXPERIMENTAL RESULTS 54

3.5 ANISOTROPIC VALENCE BAND MASSES 60

3.6 CONDUCTION BAND NONPARABOLICITY 65

3.7 OSCILLATIONS IN LINEWIDTH AND INTENSITY 68

3.8 CONCLUSIONS 73

3.9 REFERENCES 73

Chapter 4: Saturated Cyclotron Resonance 76

4.1 INTRODUCTION 77

4.2 EXPERIMENTAL SETUP 78

4.3 THE FREE ELECTRON LASER 78

4.4 THEORY 81

4.5 RESULTS AND DISCUSSION 85

4.6 CONCLUSION 88

4.7 REFERENCES 89

Chapter 5: Coupled Cyclotron Resonance 91

5.1 INTRODUCTION 92

5.2 SUBBAND-LANDAU-LEVEL-COUPLING 92

 5.2.1 *Experimental Setup* 92

 5.2.2 *Theory* 94

 5.2.3 *Results and Discussion* 98

5.3 GRATING-COUPLED CYCLOTRON RESONANCE 101

 5.3.1 *Experimental Setup* 101

 5.3.2 *Theory* 103

 5.3.3 *Results* 103

5.4 CONCLUSIONS 106

5.5 REFERENCES 107

Chapter 6: Semiconducting Superlattices 108

6.1 INTRODUCTION 109
 6.1.1 Overview 109
 6.1.2 Why InAs/GaSb? 110
6.2 LATERAL PHOTOCONDUCTIVITY 112
 6.2.1 Experiment 112
 6.2.2 Band Gap Variation with Layer Thickness 113
 6.2.3 Interband Magnetooptics 115
 6.2.4 Conclusions from Lateral Photoconductivity 121
6.3 VERTICAL PHOTOCONDUCTIVITY 122
 6.3.1 Experiment 122
 6.3.2 Results and Discussion 124
6.4 CONCLUSIONS 125
6.5 REFERENCES 125

Chapter 7: Modeling 128

7.1 MODELING THE INAS/GASB CROSSED-GAP SYSTEM 128
 7.1.1 Previous Work 128
 7.1.2 Strain 129
 7.1.3 Piezoelectric Fields 132
7.2 SEMICONDUCTING SUPERLATTICES 133
 7.2.1 Explicit interface effects 133
 7.2.2 Layer thickness fluctuation effects 137
 7.2.3 Absorption Modeling: Far-Infrared Detectors 139
7.3 SEMIMETALLIC SUPERLATTICES 143
 7.3.1 Self-Consistency 143
 7.3.2 Simplifications used in the calculations 149
 7.3.3 "Band Gaps" 150
 7.3.4 Far-Infrared Interband Detectors 153
7.4 MAGNETIC FIELDS IN INTRINSIC SYSTEMS 154
 7.4.1 Simple Model 155
 7.4.2 Multi-Band Treatment 157
 7.4.3 Magnetic Field Transitions 160
7.5 CONCLUSIONS 160
7.6 REFERENCES 160

Chapter 8: Conclusions 163

Appendix A: $k \cdot p$ Matrices 164

A.1 BLOCK-DIAGONALIZED ZERO-FIELD 4X4 HAMILTONIAN 164
A.2 ORIENTATION-DEPENDENT PARAMETERS 164
A.3 ZERO-FIELD 8X8 HAMILTONIAN FOR THE [001] GROWTH ORIENTATION 165
A.4 ZERO-FIELD 8X8 HAMILTONIAN FOR THE [111] GROWTH ORIENTATION 166
A.5 MAGNETIC FIELD 8X8 HAMILTONIAN FOR [001] AND [111] GROWTH ORIENTATIONS 167
A.6 ALL PARAMETERS USED IN THE CALCULATIONS 168



Chapter 1

Introduction

In this chapter I start with a quick outline of the scope of the thesis, then introduce the concepts and challenges involved in the physics of III-V semiconductor structures.

1.1 SCOPE OF THE THESIS.....	2
1.2 OVERVIEW.....	2
1.3 BULK MATERIALS.....	3
1.4 HETEROSTRUCTURES.....	4
1.5 THE INAS/GASB SYSTEM.....	6
1.6 GROWTH TECHNIQUES.....	8
1.7 MAGNETIC FIELD.....	9
1.8 UNITS.....	10
1.9 REFERENCES.....	10

1.1 Scope of the Thesis

This thesis is concerned with the optical properties of InAs/GaSb heterostructures under an applied magnetic field, studied in theory and experiment. As such it focuses on the properties and possible applications of this unique material system, but also provides general insight into the workings of III-V semiconductor heterostructures.

The present chapter will serve as an introduction to III-V semiconductor structures and the physics involved, and will also explain why InAs/GaSb is a system worth studying. In Chapter 2 I will illustrate some of the current quantum-mechanical models of semiconductors. One of the most common and most powerful methods for optically probing quantum electron systems is cyclotron resonance (CR), and Chapter 3 will concern itself with that. In Chapter 4, CR will be studied using extreme illumination intensities, giving details of carrier relaxation processes. The beautiful analytical simplicity of CR will be ruined in Chapter 5, where I will introduce coupling with non-CR momenta, but for good reason. Chapter 6 is an examination of thin-layer, semiconducting superlattices, with an eye for possible device applications. The final research chapter, Chapter 7, will look to the future, pushing the quantum-mechanical models of Chapter 2 to current-day limits, to predict device performance and interesting physics of the InAs/GaSb system. Chapter 8 will conclude the thesis, with a summary of the results and discussions.

1.2 Overview

Semiconductor physics has continued to grow in scope since the development of the first solid-state transistor in 1948 [1], and perhaps in no other field has application of the obscure rules of quantum mechanics led to such a dramatic impact on everyday life. Early devices were essentially replacements for vacuum tubes, but current-day devices include electro-optic switches, lasers and other devices for optical fiber and satellite communications, supercomputer processor chips, high-precision sensors, and more, all of which were unforeseen before the advent of solid state physics. The next generation of devices will undoubtedly push the limits even farther. In addition, the study of the solid state lends itself to the examination of interesting, basic physics, such as the discovery of the quantum Hall effect [2], and the phenomenon of Wigner crystallization [3].

The track record of semiconductor physics is well known and celebrated, but all researchers in the field would agree that we are still a long way from a complete understanding

of the physics of these systems, or from realizing the full potential of solid-state devices. Therefore the study of semiconducting systems continues on many fronts.

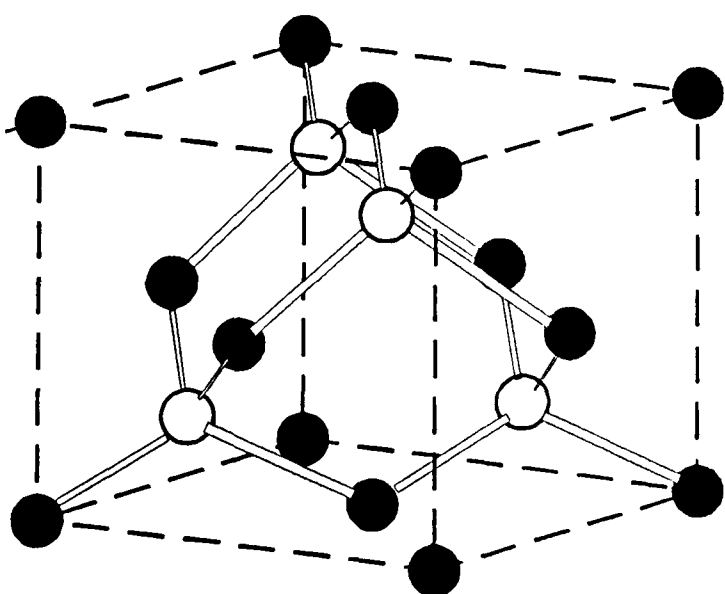
This thesis will focus on the physics of the III-V system InAs/GaSb. The ultimate goal of this research is to engineer high-temperature far-infrared detectors and emitters (lasers and light emitting diodes). Practical considerations notwithstanding, a range of interesting physics is encountered in this study, including unusual conduction and valence band-mixing effects, self-consistent electronic structure, and intense laser pulses which saturate the absorption process, to name a few examples.

1.3 Bulk Materials

An introduction to semiconductor physics, whether historical or theoretical, necessarily begins with bulk materials. It was not until pure bulk crystals were grown, studied and (partially) understood that heterostructures could be fabricated.

The characteristic feature of bulk materials is that they comprise a small unit cell of atoms, repeated with regular periodicity in all three dimensions, ideally to an infinite extent. The exact physical shape of the unit cell, and the symmetry with which it repeats, depends on the chemical nature of the constituent atoms. For III-V semiconductors the unit cell is composed of two atoms, one column-III element (Al, Ga, or In, typically) and one column-V element (P, As, or Sb). III-V semiconductors crystallize in the zincblende configuration, each element forming its own face-centered cubic (fcc) lattice, the two fcc lattices being interlaced through space (see Fig. 1.1).

The vast majority of III-V materials are covalent (with varying but slight ionic character), hence eight electrons participate in bonding. To crystallize, the outer s-levels depopulate, donating electrons to the empty p-states. The result is diamond-like tetragonal



bonds. The six occupied p-states (valence band) are nominally degenerate in energy, but split due to interaction of the angular momenta of the valence states with the crystal potential (the spin-orbit interaction). The other two electrons lie far below the valence states, in hybridized bonding s-states. The outer s-states (conduction band) are unpopulated, and sit

Figure 1.1: The zincblende crystal structure.

some energy (the band gap) above the valence states.

In reciprocal space, the zincblende structure has a truncated octagon as its first Brillouin zone. Some common high-symmetry points in the first Brillouin zone are labeled in Fig. 1.2.

Although classical mechanics can adequately describe some properties of bulk materials (e.g., the Drude model [4]), most material properties can only be described by application of quantum mechanics. To find the

electronic structure of a bulk material, one must solve Schrödinger's equation for an electron in an infinite crystal potential. Methods of solution of the wave equation are presented in Chapter 2. In general, knowing that the wave functions ψ must have the same symmetry as the crystal lattice simplifies the problem considerably. The effect of the quantizing potential of the crystal lattice is to split the free electron energy dispersion into an infinite set of discrete, quantized energy "bands." The resulting band structure for GaAs, a common III-V material, is presented in Fig. 1.3. The important detail of Fig. 1.3 is that both the conduction and valence bands have extrema at the Γ point, a characteristic feature of III-V semiconductors. Free electrons are thus likely to populate the conduction band in the region of the Γ point, and free holes will likewise populate the Γ point valence bands.

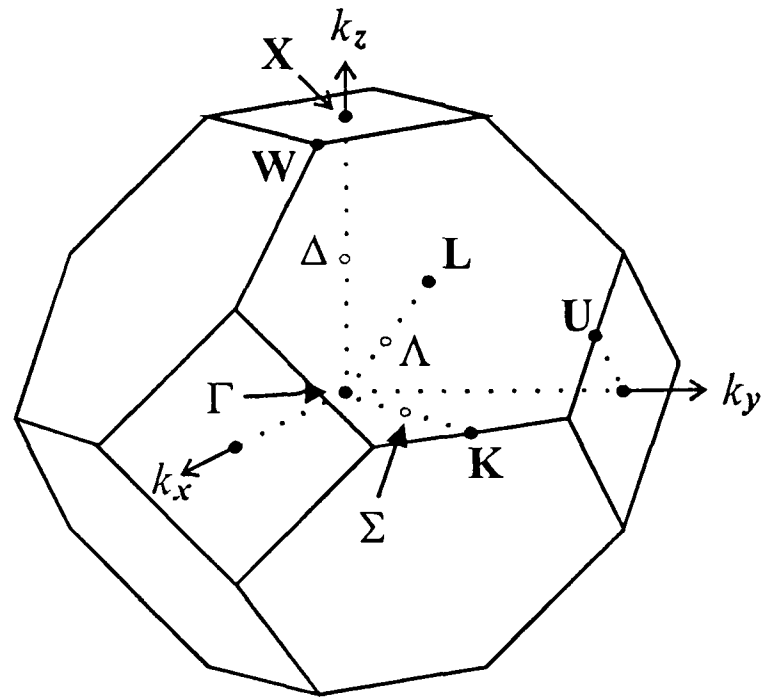


Figure 1.2: The Brillouin zone of the zincblende structure, with some high-symmetry points.

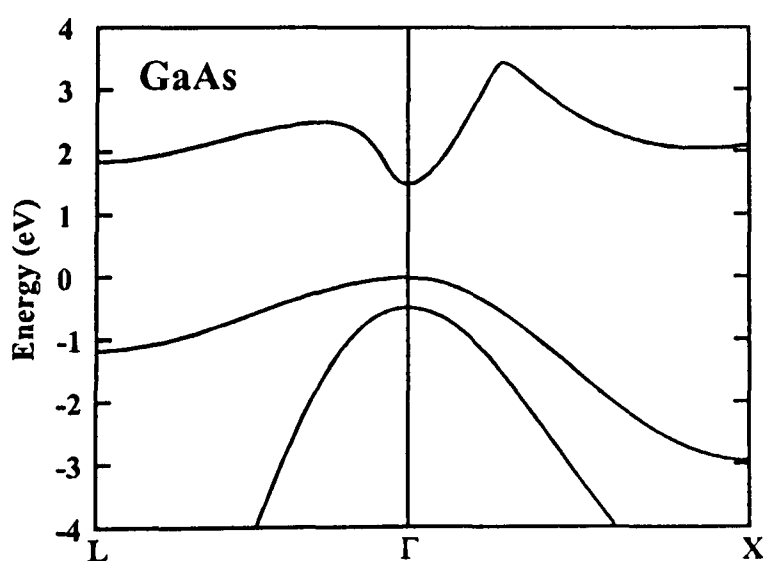


Figure 1.3: The band structure of GaAs, after Kittel [5].

1.4 Heterostructures

All of the experimental work in this thesis concerns heterostructures, the name given to a system composed of two or more distinct materials. The defining feature of heterostructures is that carriers will be strongly confined in a particular dimension, so that they exhibit two-dimensional (2D) behavior instead of the three-dimensional bulk behavior.

[Homostructures, systems composed of layers of the same material differing only in doping concentration (e.g., a p - n junction), also exhibit 2D confinement effects, but they are not studied here.]

The first heterostructures were gated Si systems, where electrons were bound in a sharp well near the metal contact, forming an “inversion layer,” or heterojunction. Other common heterostructures include quantum wells (a thin slab of one material between semi-infinite slabs, or “cladding layers,” of another material), and superlattices (repeating thin layers of different materials).

The electronic structure of a heterostructure depends in a complicated way upon the nature of the bulk materials involved. The situation is analogous to the case of a bulk crystal: in the bulk case, the free electron dispersion was split into an infinite number of energy bands, whereas in the case of a heterostructure, the additional potential splits the individual bulk energy bands into an infinite number of “subbands.” For III-V structures (or any structures with extrema at the Γ point), one can create an intuitive picture of the system by drawing the Γ -point energies as a function of position in the structure. Charge transfer and/or doping

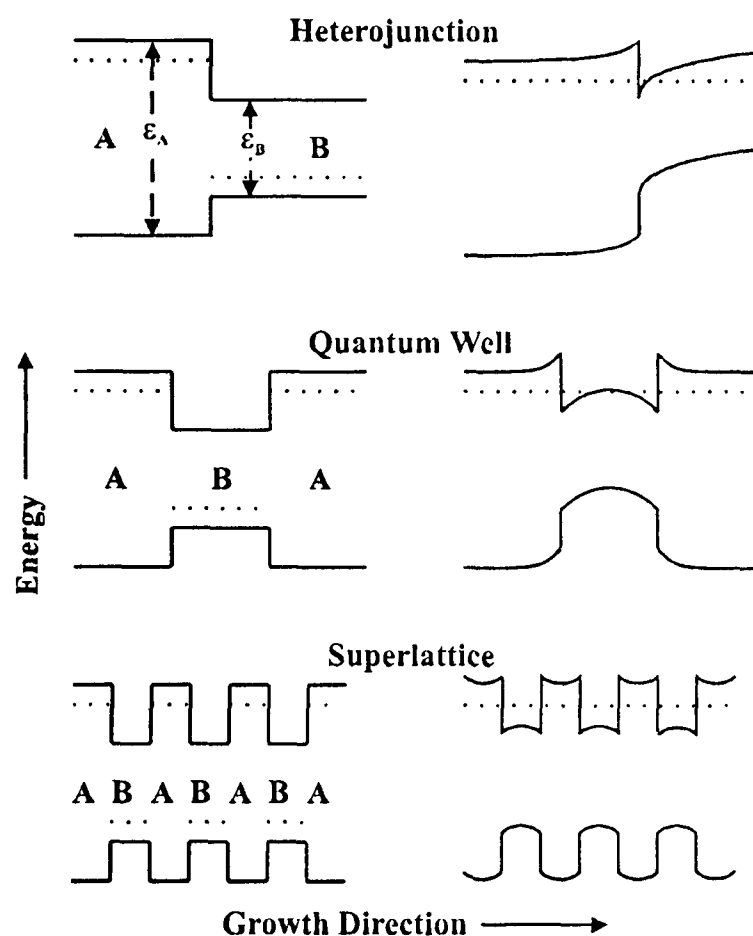


Figure 1.4: Various (Type-I) semiconductor heterostructures. Each is composed of two materials (A and B), with corresponding band gaps ϵ_A and ϵ_B . The structures on the left are the bulk band-edge lineup, with discontinuous Fermi levels. The structures on the right are at equilibrium, with stylized band-bending and a single continuous Fermi level.

effects will “bend” this band-edge potential (see Fig 1.4). In this way, the heterostructure can be thought of as a one-dimensional potential, with a corresponding one-dimensional Schrödinger wave equation.

Both quantum wells and heterojunctions confine carriers in one dimension, with the result that the free bulk momentum dispersion in that dimension is replaced by a series of discrete allowed momenta, the bound states of the confining potential. Superlattices, due to their lattice-like periodicity, still allow dispersion in the growth direction, but in a zone significantly reduced from the crystal’s Brillouin zone. Bound states exist in superlattices, as in quantum wells and heterojunctions, but each

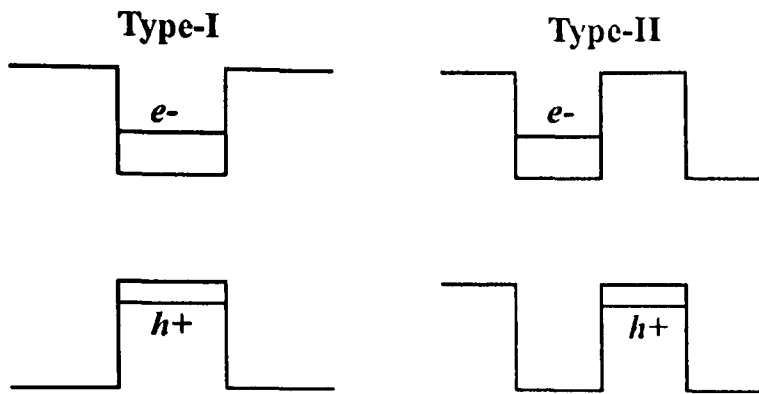


Figure 1.5: Type-I and Type-II band lineups.

state has an energy “miniband” width associated with it, as a result of the growth-direction momentum dispersion. In general the miniband width is (roughly) inversely proportional to the superlattice period.

From the line-up of the Γ -point energies, we can label heterostructures based

on their confinement effects. Structures where electrons and holes will be confined in the same layer are labeled “Type-I,” whereas structures in which electrons and holes are confined in separate layers are labeled “Type-II,” see Fig. 1.5. Type-I structures have the useful property that one can enhance inter-band transitions with the additional quantum confinement. Type-II structures cannot achieve the same degree of optical matrix-element enhancement, due to the spatial separation of carriers, but have an advantage over Type-I band line-ups in that the fundamental band gap of the structure can be less than the band gap of either constituent material. In both cases, the subband structure of the energy bands leads to interesting new phenomena, notably the integer and fractional quantum Hall effect [2,6] in transport, and intersubband transitions [7] in optical studies.

The real advantage of heterostructures is that solid state physicists now have many more variables to play with when designing devices (*i.e.*, layer widths, doping, strain, composition, *etc.*). With this “bandgap engineering” of heterostructures, one can enhance or inhibit quantum phenomena (electrical or optical properties) to a larger degree than with bulk materials.

1.5 The InAs/GaSb System

The InAs/GaSb system is a unique Type-II system, in that the valence band of GaSb lies above the conduction band of InAs (see Fig. 1.6). This “crossed-gap” feature leads to a region of energy where both electron

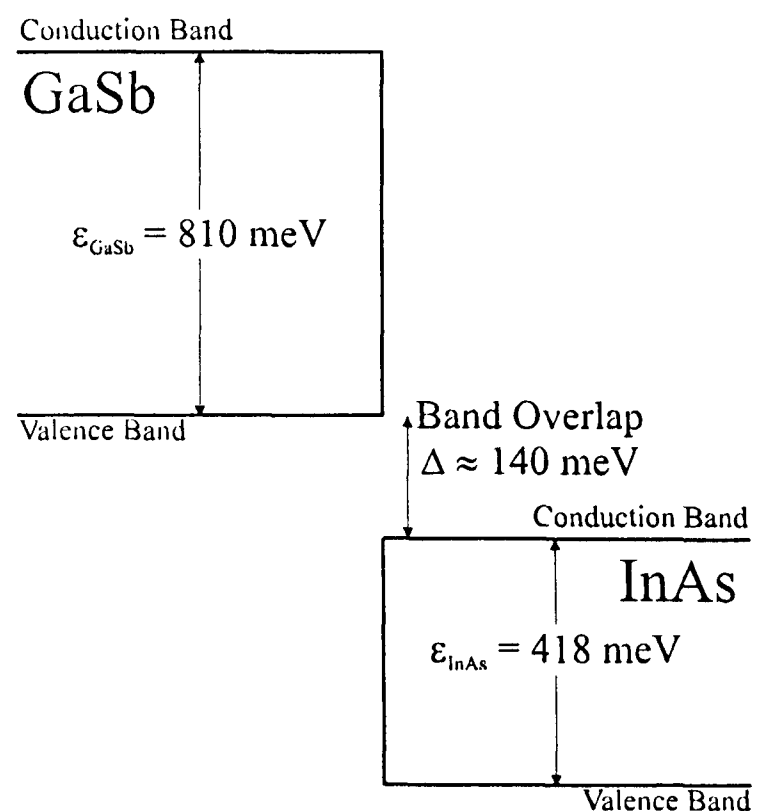


Figure 1.6: The bulk band-edge line up of InAs and GaSb. Note that the conduction band of InAs lies around 140 meV below the valence band of GaSb. This leads to a mixing of electron and hole states at the interface.

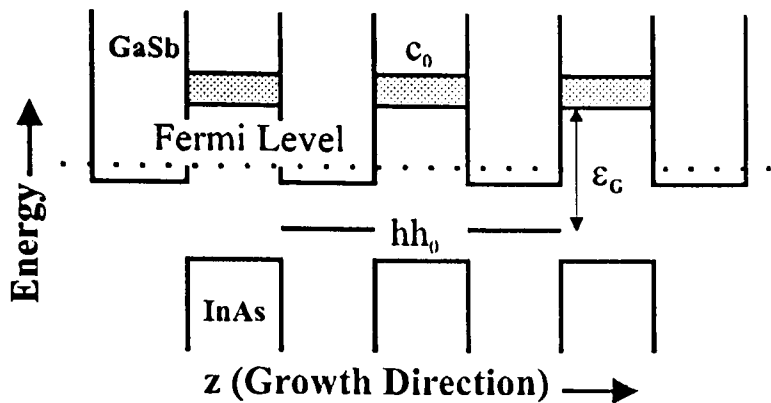


Figure 1.7: Thin-layer InAs/GaSb superlattice. The lowest-lying conduction (c_0) and heavy-hole (hh_0) states are labeled, defining a superlattice band gap (ϵ_G). The shaded area is the miniband width of the conduction level.

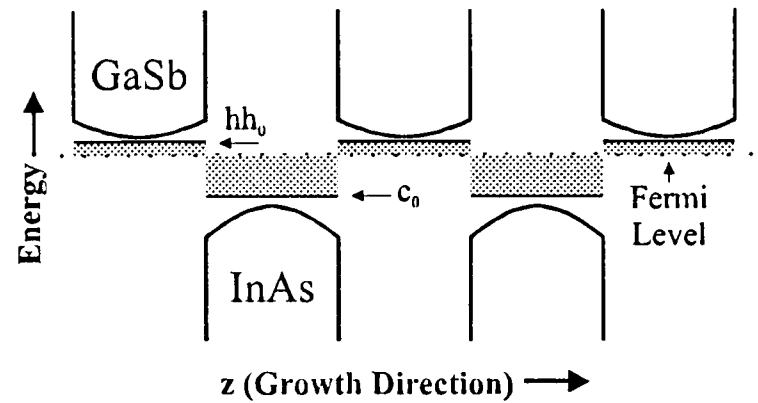


Figure 1.8: Wide-layer InAs/GaSb superlattice. The conduction band level c_0 falls below the hole level hh_0 , and the band-edges have been bent by the resulting charge transfer. The Fermi level defines electron and hole populations (shaded).

and hole states coincide. For narrow wells, confinement pushes the electron and hole levels far apart, resulting in a system with a positive band gap, like most Type-I and Type-II structures (see Fig. 1.7). Wide layer widths, however, result in the electron and hole levels settling further down into their respective energy wells, thus crossing each other. Electrons spill out from the hole level into the lower-lying electron levels, leading to a large number of intrinsic carriers at low temperatures, with no doping (see Fig. 1.8).

The amount of band overlap (the parameter Δ in Fig. 1.6) between the two materials is of considerable interest, as it determines many of the electrical and optical properties of the system. The precise value of Δ is the subject of much experimental and theoretical controversy [8-10, and references therein]. The band overlap is thought to depend on interface layer composition, growth direction (*i.e.*, [001] vs. [111]), and growth order. I do not attempt to resolve the controversy in this thesis, but I note that the data of Chapter 6 is best fitted using the band overlaps as determined by Symons *et al.* [8]. In Chapter 7, I examine the effect of interface composition in theoretical detail.

The narrow layer width system is deserving of study for its capability of near-zero band gap. This allows one to tailor devices for operation in the mid- and far-infrared regions, while avoiding problems common to other small band gap systems such as HgCdTe, notably extremely light effective masses which give rise to large tunneling currents (noise).

The wide layer width systems, with large two-carrier populations, exhibit interesting properties in transport, particularly compensated or “zeroed” Hall plateaus [11]. Optically, one can observe transitions involving both carrier types simultaneously (Chapter 3).

1.6 Growth Techniques

Heterostructures are grown by “epitaxy,” that is, the controlled growth of the structure, (ideally) laying down one atomic layer at a time, with corresponding growth rates on the order of a few Å per second. A necessary component of all epitaxial techniques is a high-quality substrate on which to grow the heterostructure, preferably lattice-matched to the heterostructure material. The samples used in this study were grown almost exclusively on GaAs substrates, although a few were grown on GaSb wafers. There are currently two major epitaxial techniques used to grow heterostructures: molecular-beam epitaxy (MBE), and a gas flow process.

MBE, as the name suggests, involves aiming beams of atoms at the growth substrate. The beams themselves are created by heating pure solid “cells” of each element, with mechanical shutters placed over the cells to control which material is grown. These beams are directed to the substrate, which is heated and kept rotating to ensure uniform deposition. The entire system, including the cell and substrate chambers, is kept at an ultra-high vacuum. By analyzing the diffraction patterns of reflected high-energy electrons (RHEED), one can monitor the growth rate and quality of the structure as it is being grown. MBE is an expensive growth technique, but it achieves very pure and controlled interfaces between materials, owing to the fast switching times of the shutters relative to the monolayer growth rate.

The gas-flow technique used at the Clarendon is metal-organic vapor-phase epitaxy (MOVPE), a process by which metal-organic molecules of the group III elements are mixed with hydrides (organic compounds) of the group V elements, and passed over a heated substrate [12,13]. Due to the gas flow in the growth chamber (pressures of order 1 bar), RHEED cannot be used, but recently Mason and Walker [14] have circumvented this problem by monitoring the UV absorption line of particular alkyls, which gives a measurement of the concentration of precursors entering the growth chamber. MOVPE is much less expensive than MBE, although the interfaces between material layers is usually several monolayers wide. Nonetheless, for InAs/GaSb structures, the MOVPE-grown samples of the Clarendon have almost perfectly intrinsic carrier concentrations, unlike MBE samples which are predominantly n-type [15-17].

1.7 Magnetic Field

As the title of the thesis suggests, magnetic fields play an important role in the experiments presented here. Given that the aim of this research is devices which perform at high temperatures in absence of field, it may seem incongruous to have performed all these experiments under vacuum at 4K or colder, with superconducting magnets providing fields up to 17 Tesla.

Obviously, the direct answer is simply that as basic research, experimental results are easier to analyze when not complicated by atmospheric absorption, condensation, or heating effects. The use of cryogenics in semiconductor research has proven so successful that it needs no defense here, but I will mention one more aspect of the use of magnetic field. In a similar manner as the bulk crystal potential quantized and “split” the free-electron dispersion, and as the heterostructure potential quantized and split the bulk energy bands, so a growth-direction magnetic field quantizes and splits the heterostructure subbands into Landau levels (see Fig. 1.9). Furthermore, transitions between adjacent Landau levels are strong, meaning that even when the heterostructure subbands do not couple strongly, transitions may be observed when a field is applied (the mechanics of transition matrix elements are discussed in Chapter 2). In effect, the extra degree of quantization provided by the magnetic field enhances the quantum properties of the heterostructure.

This extra quantization is an extremely useful property, and is what makes magnetic fields such powerful tools for the experimentalist. The experimental setup changes little from chapter to chapter: basically the sample is placed with light and magnetic field perpendicular to the planes of the layers. Yet a magnetic field, coupled with a few extra external variables, yields a rich variety of behavior, and allows a thorough investigation of the electronic structure of the system.

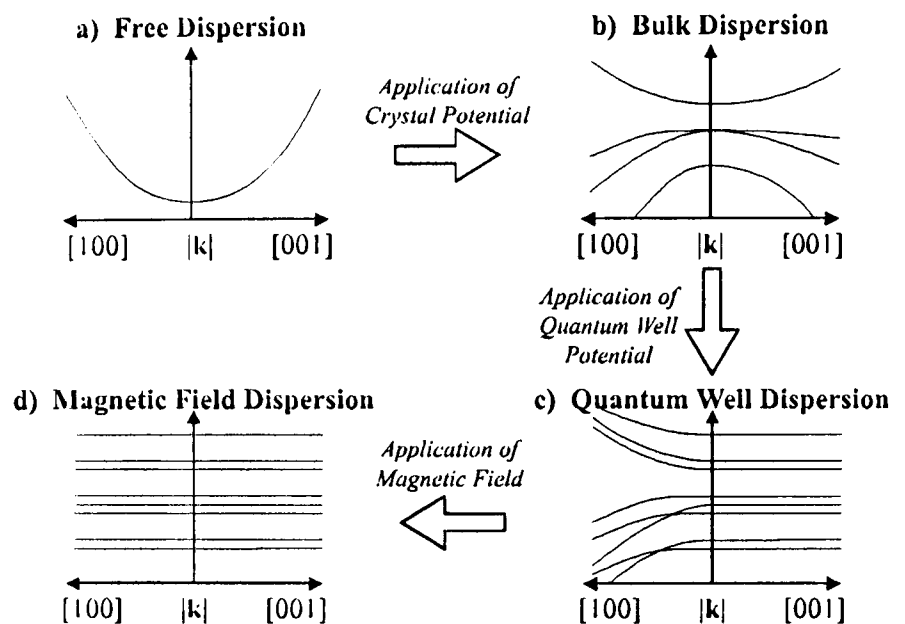


Figure 1.9: The path to complete quantization. In a), all energy states (above $|k| = 0$) are available to the electron. In b), the crystal potential breaks the bulk dispersion into energy bands. In c), the bulk bands are split into subbands with uniquely determined k_z values. These quantum well subbands are completely quantized in d), with the application of a magnetic field. In d), the bands are shown for fixed field and Landau level index.

Table 1.1: The fundamental and derived constants in atomic and SI units (from ref. [18]).

Quantity	Symbol	Atomic Units	SI Units
Fundamental Constants			
Planck's Constant $\hbar/2\pi$	$\hbar$	1	1.05459×10^{-34} Js
Proton Charge	e	1	1.60219×10^{-19} C
(no name)	$4\pi\epsilon_0 = \kappa_0$	1	$4\pi \times 8.85420 \times 10^{-12}$ Fm ⁻¹
Electron Rest Mass	m_0	1	9.10956×10^{-31} kg
Derived Constants			
Energy	Hartree (H)	1	27.2112 eV
Length	Bohr radius (a_0)	1	0.529177 Å
Magnetic Field	Atomic Tesla (aT)	1	2.35053×10^5 T
Time	Atomic Second (as)	1	2.41889×10^{-17} s
Speed of Light	c	$1/\alpha \approx 137$	2.997925×10^8 m/s

1.8 Units

When performing any kind of calculation or computer modeling, the choice of units is important to ensure consistency. I have chosen the system of atomic units [18], where the fundamental constants $\hbar$, e , κ_0 , and m_0 are all set to unity (see Table 1.1). With these four parameters established, one can derive any other parameter solely by consideration of the units involved. Some common derived units (and their SI equivalent) are presented in Table 1.1 as well.

Atomic units are particularly useful for semiconductor modeling, as most physical parameters are expressed in numbers on the order of unity. In addition, almost all formulae are clear functions of variables such as applied field, effective mass, *etc.*, without being cluttered by physical constants. Theoretical calculations are simplified considerably (and hence are more stable) by using atomic units, and the equations themselves are faster and more intuitive to manipulate.

1.9 References

- [1] J. Bardeen and W. H. Brattain, Phys. Rev. **74** (1948) 230.
- [2] K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45** (1980) 494.
- [3] J. Michels, *D.Phil. Thesis*, (1994).
- [4] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Holt, Rinehart and Winston, New York, 1976.
- [5] C. Kittel, *Introduction to Solid State Physics*, 6th ed., John Wiley & Sons, New York, 1986.

- [6] D. R. Leadley, R. J. Nicholas, C. T. Foxon, and J. J. Harris, Phys. Rev. Lett. **72** (1994) 1906.
- [7] C. Weisbuch and B. Vinter, *Quantum Semiconductor Structures: Fundamentals and Applications*, Academic Press, London, 1991.
- [8] D. M. Symons, M. Lakrimi, R. J. Warburton, R. J. Nicholas, N. J. Mason, P. J. Walker, and M. I. Eremets, Semicond. Sci. Tech. **9** (1994) 118.
- [9] D. M. Symons, M. Lakrimi, M. van der Burgt, T. A. Vaughan, R. J. Nicholas, N. J. Mason, and P. J. Walker, Phys. Rev. B **51** (1995) 1729.
- [10] J. R. Waterman, B. V. Shanabrook, R. J. Wagner, M. J. Yang, J. L. Davis, and J. P. Omaggio, Semicond. Sci. Tech. **8** (1993) S106.
- [11] M. S. Daly, K. S. H. Dalton, M. Lakrimi, N. J. Mason, D. K. Maude, R. J. Nicholas, J. C. Portal, D. M. Symons, M. van der Burgt, and P. J. Walker, submitted to Phys. Rev. Lett., August 1995.
- [12] G. R. Booker, P. C. Klipstein, M. Lakrimi, S. Lyapin, N. J. Mason, R. J. Nicholas, T.-Y. Seong, D. M. Symons, T. A. Vaughan, and P. J. Walker, J. Crystal Growth **145** (1994) 778.
- [13] G. R. Booker, P. C. Klipstein, M. Lakrimi, S. Lyapin, N. J. Mason, I. J. Murgatroyd, R. J. Nicholas, T.-Y. Seong, D. M. Symons, and P. J. Walker, J. Crystal Growth **146** (1995) 495.
- [14] N. J. Mason and P. J. Walker, to be published.
- [15] J. Beerens, G. Grégoris, J. C. Portal, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **36** (1987) 4742.
- [16] J. R. Meyer, C. A. Hoffman, B. V. Shanabrook, B. R. Bennett, R. J. Wagner, J. R. Waterman, and E. R. Youngdale, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, World Scientific, Singapore, 1995, p. 783.
- [17] L. S. Kim, H. D. Drew, H. Munekata, L. L. Chang, and L. Esaki, Solid State Comm. **66** (1988) 873.
- [18] R. McWeeny, Nature **243** (1973) 196.

Chapter 2

$k \cdot p$ Theory and the Envelope Function Approximation

In this chapter I present the basic concepts of $k \cdot p$ theory and the envelope function approximation (EFA), particularly as applied to the III-V system of InAs/GaSb. $k \cdot p$ theory is a method of calculating the electronic structure (energy levels and wave functions) of electrons in crystal lattices, and can be extended via the EFA to apply to heterostructures as well. The methods described here form the backbone of much later analysis, as in general observable properties of heterostructures are straightforward to calculate once the electronic structure is known.

2.1 BULK LATTICES: $K \cdot P$ THEORY.....	13
2.1.1 FRAMEWORK OF $K \cdot P$ THEORY.....	13
2.1.2 SOLVING FOR BULK EIGENSTATES	15
2.1.3 EXPANDING AROUND A SPECIAL POINT IN THE BRILLOUIN ZONE	15
2.1.4 CONSTRUCTING BULK HAMILTONIANS.....	16
2.2 HETEROSTRUCTURES: THE ENVELOPE FUNCTION APPROXIMATION.....	21
2.2.1 FRAMEWORK OF THE ENVELOPE FUNCTION APPROXIMATION.....	21
2.2.2 THE TRANSFER-MATRIX TECHNIQUE.....	28
2.2.3 THE “MOMENTUM-MATRIX” TECHNIQUE	34
2.2.4 CHOICE OF A BASIS SET	38
2.3 APPLICATION OF MAGNETIC FIELD	39
2.4 OBSERVABLES: TRANSITIONS AND SELECTION RULES.....	41
2.4.1 ZERO MAGNETIC FIELD	42
2.4.2 APPLIED MAGNETIC FIELD	43
2.4.3 TYPE-I VERSUS TYPE-II SELECTION RULES	43
2.4.4 INFLUENCES OF FAR BANDS	44
2.5 FINAL NOTE	45
2.6 REFERENCES	45

2.1 Bulk Lattices: $k \cdot p$ Theory

$k \cdot p$ theory was first constructed forty years ago to explain cyclotron resonance in bulk materials [1]. Since then it has grown to become the method of choice for physicists who model semiconductors, having been spectacularly successful in explaining experimental results [2]. The derivation of the $k \cdot p$ model has been well explained by Kane [3] and others [1,4,5], but my objective in this chapter is to explain the basics of $k \cdot p$ theory, particularly those aspects which proved to be useful when dealing with heterostructures and the EFA later in the chapter. I shall highlight the major results and limitations of both models.

In this chapter I follow convention and use atomic units (discussed in Chapter 1), and so the constants $\hbar$, e , m_0 , and κ_0 ($4\pi\epsilon_0$) are unity and have been dropped from all equations.

2.1.1 Framework of $k \cdot p$ Theory

The aim of modeling is to determine the energies and wave functions of electrons inside the semiconductor. Therefore, the problem requires a solution of the time-independent Schrödinger wave equation (SWE) in the absence of applied magnetic field

$$\left[\frac{p^2}{2} + V(r) + \frac{1}{4c^2} (\nabla V \times p) \cdot \sigma \right] \psi = E \psi, \quad (2.1)$$

for a three-dimensional, infinite crystal potential $V(r)$. The first term in Eq. (2.1) is the kinetic energy operator, and the third term accounts for the spin-orbit splitting of the energy states. Here σ is the Pauli spin operator, with elements

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.2)$$

Obviously, one cannot hope to solve the SWE by modeling the lattice physically, with Coulomb potentials attached to each nuclear core. Instead, the symmetry of the crystal lattice is exploited to provide clues as to the solutions.

The first tool employed in the solution of Eq. (2.1) is the Bloch (or Floquet) theorem. It is a fundamental mathematical result that solutions ψ of periodic, linear differential equations must have the property

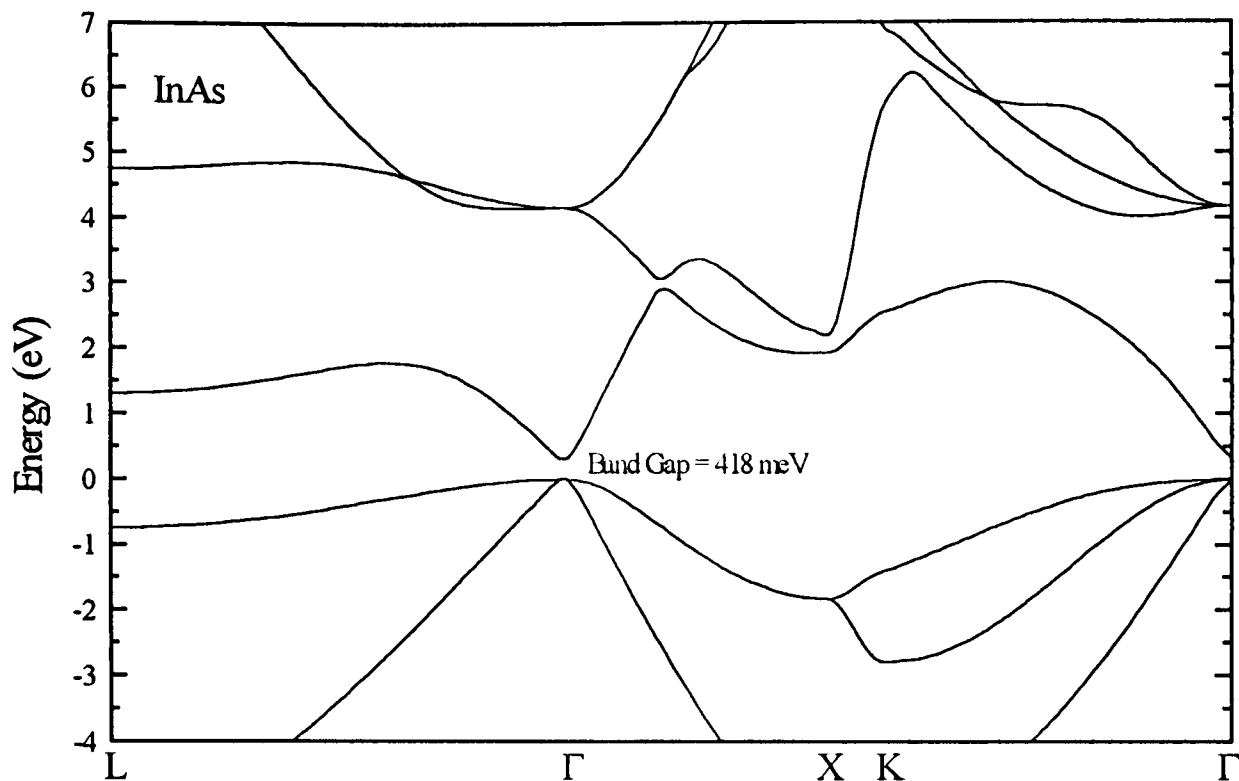


Figure 2.1: The band structure of bulk InAs, calculated from the pseudopotential technique of ref. 6.

$$\psi(\mathbf{r}+\mathbf{t}) = e^{i\mathbf{k}\cdot\mathbf{t}} \psi(\mathbf{r}), \quad (2.3)$$

where $\mathbf{t}$ is a translation vector such that $V(\mathbf{r}+\mathbf{t}) = V(\mathbf{r})$, and $\mathbf{k}$ is a phase constant. In the physical case of a crystal lattice, $\mathbf{t}$ corresponds to any spatial translation with the periodicity of the unit cell of the crystal, and $\mathbf{k}$ to the momentum wave vector $\mathbf{k} = (k_x, k_y, k_z)$. Eq. (2.3) can be re-written as a constraint on the wave function $\psi(\mathbf{r})$:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} |u_{\mathbf{k}}(\mathbf{r})\rangle, \quad (2.4)$$

where I have introduced the Dirac bra-ket notation for the function $u_{\mathbf{k}}(\mathbf{r})$. Eq. (2.4) states that any wave function satisfying the SWE will be composed of two distinct parts: a phase factor depending on the momentum of the state (the $e^{i\mathbf{k}\cdot\mathbf{r}}$ term), and a “Bloch function” with the periodicity of the lattice (hence $|u_{\mathbf{k}}(\mathbf{r}+\mathbf{t})\rangle = |u_{\mathbf{k}}(\mathbf{r})\rangle$). As said before, the Bloch theorem is a fundamental property of periodic linear differential equations, a property that will be used again in heterostructure superlattices.

At this point, knowing nothing about the Bloch functions except for their invariance under lattice translation, Eq. (2.4) is substituted back into the SWE to find

$$\left[\frac{k^2}{2} + \mathbf{k}\cdot\mathbf{p} + \frac{p^2}{2} + V(\mathbf{r}) + \frac{1}{4c^2} (\nabla V \times (\mathbf{k} + \mathbf{p})) \cdot \boldsymbol{\sigma} \right] |u_{\mathbf{k}}(\mathbf{r})\rangle = E |u_{\mathbf{k}}(\mathbf{r})\rangle, \quad (2.5)$$

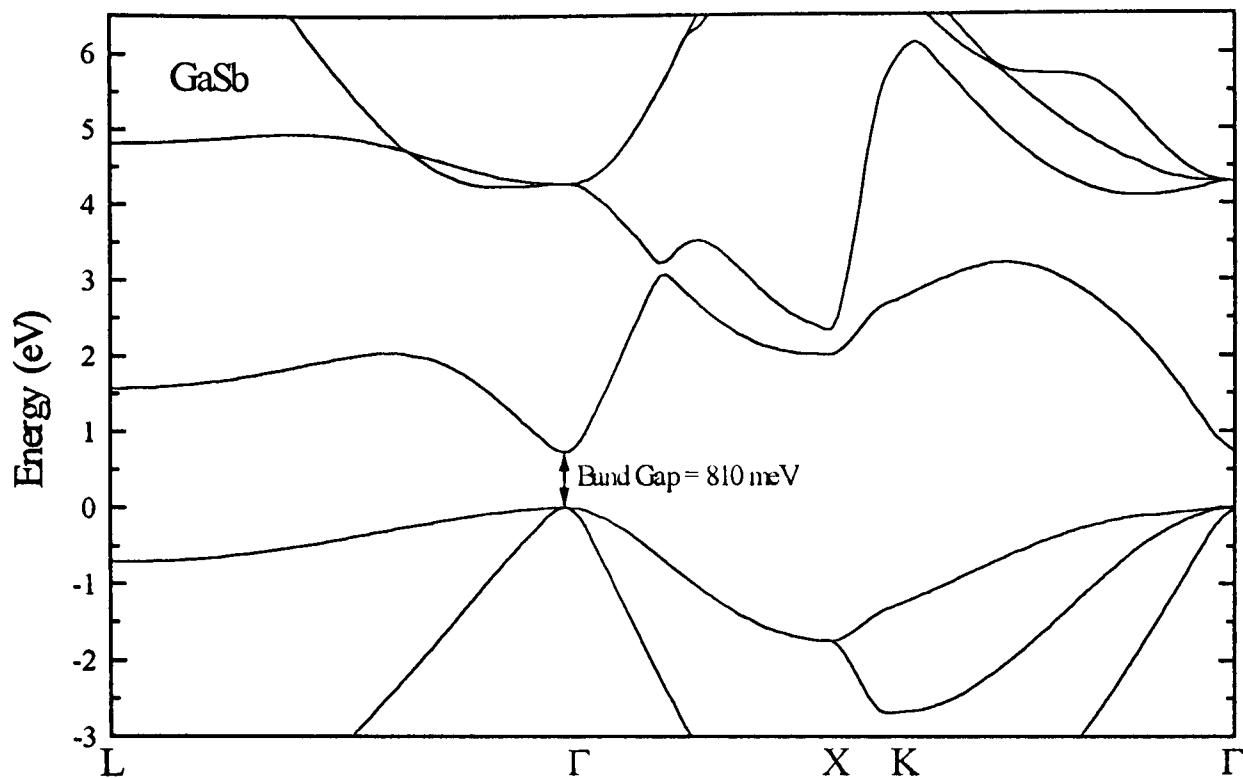


Figure 2.2: The band structure of GaSb, calculated from the pseudopotential technique of ref. 6.

which is the equation defining the Bloch states $|u_k(\mathbf{r})\rangle$.

2.1.2 Solving for Bulk Eigenstates

From Eq. (2.5), one can calculate the energies E and wave functions $|u_k(\mathbf{r})\rangle$ of a bulk crystal given the momentum $\mathbf{k}$. In practice, one deduces the form of $V(\mathbf{r})$ from the crystal symmetry and experimentally observed energy splittings, and then composes the eigenstates as a linear superposition of plane waves with the periodicity of the lattice (this is the pseudopotential technique, see ref. [6]). The band structures of InAs and GaSb have been calculated this way, and are presented in Figs. 2.1 and 2.2 (where the spin-orbit splitting has been neglected). The symmetry points of the Brillouin zone are labeled in Fig. 1.2.

2.1.3 Expanding around a Special Point in the Brillouin Zone

The Bloch functions $|u_k(\mathbf{r})\rangle$ are a complete, orthogonal set of functions, and so span the entire set of functions with the periodicity of the crystal lattice. It is therefore convenient to select a particular point in the Brillouin zone $\mathbf{k}_0$, and expand all solutions of Eq. (2.5) for general $\mathbf{k}$ as a linear superposition of the states at $\mathbf{k}_0$. In particular, states $|u_k(\mathbf{r})\rangle$ can be adequately described by only a few $|u_{\mathbf{k}_0}(\mathbf{r})\rangle$ states if $\mathbf{k}$ is sufficiently close to $\mathbf{k}_0$.

To select a $\mathbf{k}_0$ point, one considers which $\mathbf{k}$ -point in the crystal is the most “interesting,” defined as the point where most free carriers (electrons or holes) are likely to

reside. For III-V crystals, the Γ point ($k_0 = 0$) is the location of both the conduction and valence band extrema (as is evident in Figs. 2.1 and 2.2 above). The band extrema are the most likely k points to be populated given finite temperature or doping effects.

Having chosen the Γ point as the point in k -space to expand around, an energy scale is now determined. There are an infinite number of states available to carriers at the Γ point, but only the few which are most likely to be occupied are selected. These are the doubly-degenerate conduction states ($|s\rangle$ with spin $\uparrow$ and spin $\downarrow$) and the six-fold degenerate valence states ($|x\rangle$, $|y\rangle$, and $|z\rangle$, again with spins $\uparrow$ and $\downarrow$, where I have neglected the spin-orbit splitting in discussing degeneracies). For the rest of this thesis, I therefore expand all bulk solutions in terms of these eight Γ states, and their associated energies.

If necessary, one can solve Eq. (2.5) at the Γ point to find the exact physical form of the eigenstates. In practice, one determines the eigenenergies from experimental data, and uses the symmetries of the wave functions rather than their exact functional form when constructing bulk Hamiltonians.

At this point, the crucial approximations of $k \cdot p$ theory have been made, and so one can evaluate its limitations. By choosing as a basis the eight Γ s and p states, the range of investigation has been restricted to those momentum states near the center of the Brillouin zone, with energies near the fundamental energy gap of the crystal. The question is: does this restrict the usefulness of the theory?

The answer is no, the theory is in fact extremely useful for III-V semiconductors. How can only eight states serve to describe the system so well? For the vast majority of physical phenomena considered, carriers will remain near the Γ point, and will not stray far in energy from the band gap. Therefore, any state likely to be populated may be accurately expressed as a linear combination of the Γ basis functions.

2.1.4 Constructing Bulk Hamiltonians

The eight basis states having been chosen, the mathematical machinery necessary to expand states near the Γ point is constructed. The standard approach for bulk modeling is to write general states $|u_{nk}(\mathbf{r})\rangle$ as linear combinations of the Γ states $|u_{n\Gamma}(\mathbf{r})\rangle$. With an eye to the EFA formalism presented later, however, I write the wave function $\psi(\mathbf{r})$ as a combination of the Bloch states modulated with some unspecified function $f(\mathbf{r})$, as

$$\psi(\mathbf{r}) = \sum_j^{\Gamma} f_j(\mathbf{r}) |u_{j\Gamma}(\mathbf{r})\rangle, \quad (2.6)$$

where, for the moment, the sum is over *all* Γ states.

To ease the discussion of applied magnetic field, I introduce the full Hamiltonian for arbitrary field

$$H = \frac{\mathbf{P}^2}{2} + V(\mathbf{r}) + \mu_B \mathbf{B} \cdot \boldsymbol{\sigma} + \frac{1}{4c^2} (\nabla V \times \mathbf{P}) \cdot \boldsymbol{\sigma}, \quad (2.7)$$

where μ_B is the Bohr magneton and $\mathbf{P}$ is the momentum operator

$$\mathbf{P} = \mathbf{p} + \mathbf{A}, \quad (2.8)$$

with vector potential $\mathbf{A}$ and corresponding magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. The basis functions are still the Bloch functions $|u_{j\Gamma}(\mathbf{r})\rangle$, which are eigenstates of the Hamiltonian of Eq. (2.5). The effects of the vector potential $\mathbf{A}$, and spin splitting $\mathbf{B} \cdot \boldsymbol{\sigma}$, are therefore included as a perturbation, in the same way as the finite wave vector $\mathbf{k}$.

Assuming a vector potential of Landau gauge (such that $\nabla \cdot \mathbf{A} = 0$), one operates upon the wave function of Eq. (2.6) with the Hamiltonian of Eq. (2.7), and integrates over a unit cell with Bloch basis function $\langle u_{i\Gamma}(\mathbf{r}) |$ to find the eigenequation

$$\sum_j^{\Gamma} H_{ij} f_j = E_j f_j, \quad (2.9)$$

where the Hamiltonian elements are defined

$$H_{ij} = \left[E_j^{(0)} + \frac{\mathbf{P}^2}{2} \right] \delta_{ij} + \Pi_{ij} \cdot \mathbf{P} + \mu_B \mathbf{B} \cdot \boldsymbol{\sigma}_{ij}, \quad (2.10)$$

where μ_B is the Bohr magneton, $E_j^{(0)}$ is the energy of basis state j at $\mathbf{k} = 0$, and the Kane matrix element Π_{ij} is defined

$$\Pi_{ij} = \langle u_{i\Gamma} | \mathbf{p} + \frac{1}{4c^2} (\boldsymbol{\sigma} \times \nabla V) | u_{j\Gamma} \rangle. \quad (2.11)$$

Unfortunately, the matrix H of Eq. (2.10) is infinite in extent. To reduce the Hamiltonian to a manageable size, only the eight s and p states are explicitly included. Rather than dropping all effects of far Γ states, their influences are included perturbatively. This is done using Löwdin perturbation theory [1,3], where the interactions between the selected basis states are renormalized as a result of removing explicit interactions with farther bands. The renormalized matrix elements have the form

$$h'_{ij} = h_{ij} + \sum_l^{\Gamma'} \frac{h_{il} h_{lj}}{E_i^{(0)} - E_l^{(0)}}, \quad (2.12)$$

where Γ' denotes the set of Γ states not included in the basis states, i and j are basis states, and l is in Γ' . Löwdin perturbation is valid so long as the interaction terms h_{il} are much smaller than the energy differences between the states $E_i^{(0)} - E_l^{(0)}$. For III-V semiconductors, the far states are several band gaps away in energy, hence the perturbation is accurate. The effect of Eq. (2.12) is to add new terms to the Hamiltonian elements h_{ij} , terms which account for the influences of far away bands.

The wave function coefficients of far bands in Eq. (2.6) are now of the form

$$f_l(\mathbf{r}) = \sum_j \frac{h_{lj}}{E_j^{(0)} - E_l^{(0)}} f_j(\mathbf{r}), \quad (2.13)$$

for l in Γ' , and j in the set of included basis states. When looking at optical transitions, this mixing with far Γ states becomes important.

Including the Löwdin perturbation of Eq. (2.12) with the Hamiltonian of Eq. (2.10) the renormalized Hamiltonian elements are given by

$$H_{ij} = E_j^{(0)} \delta_{ij} + \Pi_{ij} \cdot \mathbf{P} + \mu_B \mathbf{B} \cdot \boldsymbol{\sigma}_{ij} + \sum_{\alpha, \beta} D_{ij}^{\alpha\beta} P_\alpha P_\beta, \quad (2.14)$$

where the effective mass tensor $D_{ij}^{\alpha\beta}$ is defined

$$D_{ij}^{\alpha\beta} = \frac{1}{2} \delta_{ij} \delta_{\alpha\beta} + \sum_l^{\Gamma} \frac{\Pi_{il}^{\alpha} \Pi_{lj}^{\beta}}{E_i - E_l}, \quad (2.15)$$

with $\alpha, \beta \in \{x, y, z\}$. Here the spin-splitting term in the Löwdin perturbation has been dropped, as it is a small correction to the momentum element Π_{ij} . In practice, when determining the tensor of Eq. (2.15), one uses the symmetry of the i, j states to determine which elements are nonzero, then applies experimentally observed splittings and effective masses to fit the nonzero terms. Less commonly, the exact functional form of the wave functions can be determined from Eq. (2.5), and then the terms of Eq. (2.15) are calculated explicitly.

The basis set, when written as linear combinations of the Γ -point s and p states, is the familiar Kane Γ states with associated eigenenergies as presented in Table 2.2, where E_G is the band gap energy, Δ is the spin-orbit splitting of the p -states given by

$$\Delta = -\frac{3i}{4c^2} \langle x | \nabla V \times \mathbf{p} | z \rangle, \quad (2.16)$$

Table 2.2: The Γ -point $[001]$ Kane basis set.

	$ j, m_j\rangle$	ψ_{jm}	E_{Γ}
c $\uparrow$	$ ^{1/2}, +^{1/2}\rangle$	$ s\uparrow\rangle$	E_G
hh $\uparrow$	$ ^{3/2}, +^{3/2}\rangle$	$\frac{1}{\sqrt{2}}(i x\uparrow\rangle + y\uparrow\rangle)$	0
lh $\downarrow$	$ ^{3/2}, -^{1/2}\rangle$	$\frac{1}{\sqrt{6}}(i x\uparrow\rangle - y\uparrow\rangle - 2i z\downarrow\rangle)$	0
so $\downarrow$	$ ^{1/2}, -^{1/2}\rangle$	$\frac{1}{\sqrt{3}}(i x\uparrow\rangle - y\uparrow\rangle + i z\downarrow\rangle)$	$-\Delta$
c $\downarrow$	$ ^{1/2}, -^{1/2}\rangle$	$ s\downarrow\rangle$	E_G
hh $\downarrow$	$ ^{3/2}, -^{3/2}\rangle$	$\frac{1}{\sqrt{2}}(i x\downarrow\rangle - y\downarrow\rangle)$	0
lh $\uparrow$	$ ^{3/2}, +^{1/2}\rangle$	$\frac{1}{\sqrt{6}}(i x\downarrow\rangle + y\downarrow\rangle + 2i z\uparrow\rangle)$	0
so $\uparrow$	$ ^{1/2}, +^{1/2}\rangle$	$\frac{1}{\sqrt{3}}(i x\downarrow\rangle + y\downarrow\rangle - i z\uparrow\rangle)$	$-\Delta$

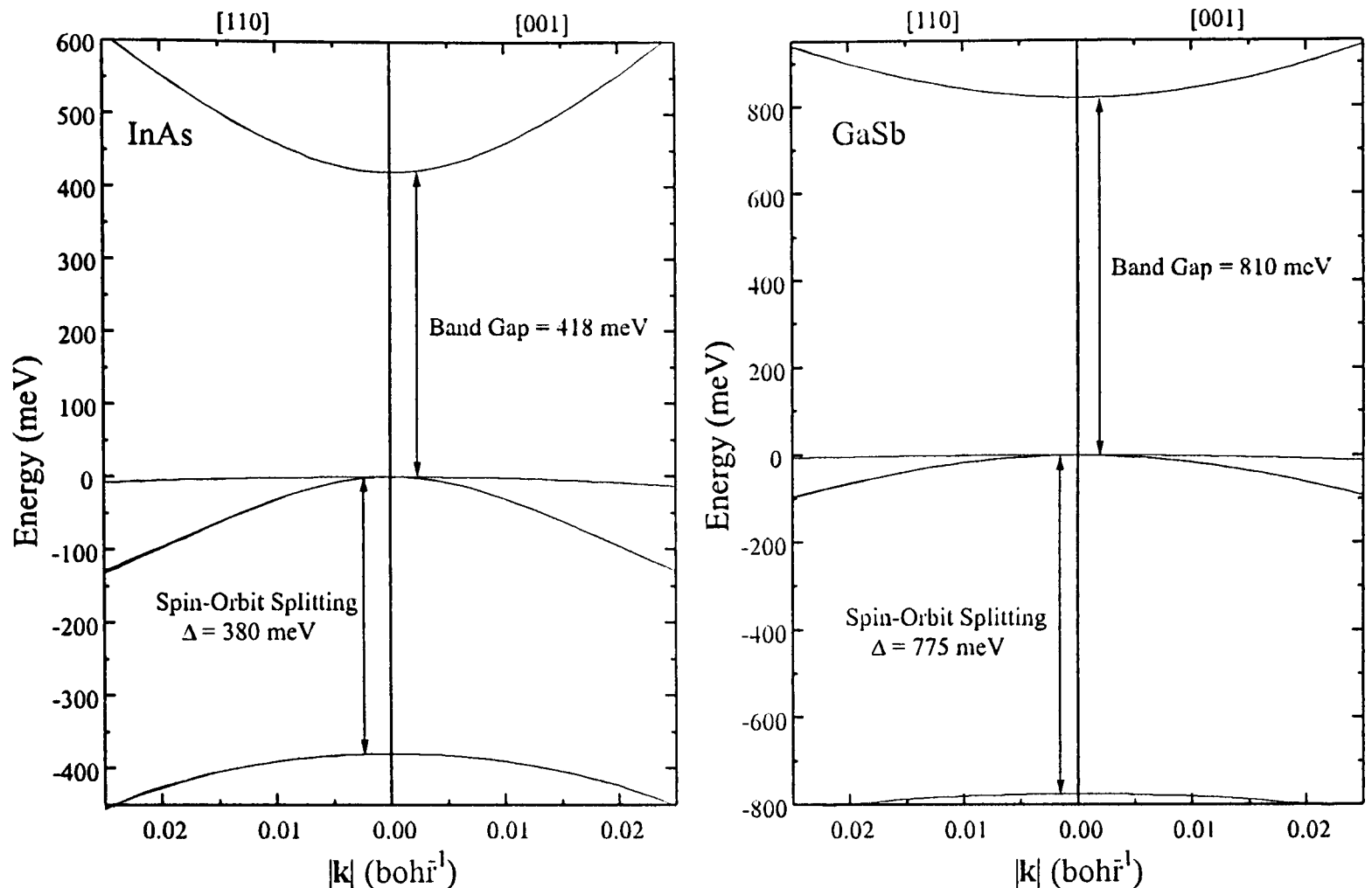


Figure 2.3: Energy band dispersions of InAs and GaSb near the Γ -point, calculated by diagonalization of the bulk $\mathbf{k}\cdot\mathbf{p}$ matrix for each material. The matrices were computed directly, using the pseudopotential method of ref. [6] and formalism of ref. [7].

and the zero of energy is defined to be at the valence band edge.

I refer to the eight basis states used in construction of the bulk Hamiltonian as the “Kane basis.” The Kane states themselves are linear combinations of the “Bloch functions,” the atomic s and p states with corresponding spin. The terminology becomes important--and confusing--when dealing with non-[001] growth directions, as there the Kane states are linear superpositions of linear superpositions of Bloch functions.

The bulk Hamiltonian matrices can then be calculated with the basis states of Table 2.2 and the Hamiltonian matrix of Eq. (2.14). In practice, this is a tedious bit of algebra which is best left to a computer. Appendix A gives the 8x8 bulk Hamiltonian constructed in this manner (the [001] Hamiltonian).

To determine the bulk electronic structure for a given $\mathbf{k}$ point close to Γ , one diagonalizes the bulk Hamiltonian matrix at that $\mathbf{k}$ -value (with no applied field, the $\mathbf{P}$ operator may be replaced by $\mathbf{k}$, as the carriers move freely in all directions). The eigenvalues of the matrix are the eigenenergies of the states, and the eigenvectors give the coefficients of the Kane states of Table 2.2. Solving for the electronic structure in this manner is orders of

magnitude faster than solving Eq. (2.5) explicitly, and is just as accurate for k close to Γ . The bulk dispersion curves for InAs and GaSb are presented in Fig. 2.3.

The effective mass tensor of Eq. (2.15) contains much of the symmetry information about the crystal. It is what gives rise to band curvature terms such as F , γ_1 , γ_2 , and γ_3 in the bulk Hamiltonians. In III-V materials, the lack of inversion symmetry gives rise to additional curvature terms. However, I have assumed inversion symmetry throughout, also known as the “Germanium approximation” [4]. Weiler [4] gives the full 8-band bulk [001] Hamiltonian with all symmetry-breaking terms (her Table II). If one ignores the symmetry-breaking terms our Hamiltonians match. These symmetry breaking terms are often dropped [3,5], as they are thought to be small, and the band structure can be well-described by the fewest possible number of parameters.

2.2 Heterostructures: The Envelope Function Approximation

The EFA is a method of extending $k \cdot p$ theory to apply to semiconductor heterostructures. The main feature of the method is that it makes one assumption regarding the form of the wave function in a heterostructure, an assumption which renders it possible to calculate the electronic structure.

Although the methods here are general, in that they can be applied to any heterostructure, this thesis concerns itself with superlattices. Therefore the solutions presented below have been derived from superlattice boundary conditions. Fortunately, this is not much of a limitation, since quantum well and heterojunction structures can be represented as superlattices with large layer widths. Alternatively, it is a relatively simple matter to reformulate the methods below to apply to quantum well or heterojunction boundary conditions.

2.2.1 Framework of the Envelope Function Approximation

At first glance, the problem of solving for the electronic structure of a semiconductor heterostructure seems almost intractable. As in the bulk case, a carrier moving through the structure would see an infinite number of nuclear cores. Unlike the bulk case, however, the symmetry of the problem is broken by the heterostructure, as different layers of material alter the form of the crystal lattice in different locations.

This problem is circumvented by making a simplifying assumption about the wave function: it is assumed that the wave function will be a linear superposition of the Kane basis states, as before, but this superposition is modulated with a slowly-varying envelope function,

to account for the confining effects of the heterostructure (“slowly-varying” requires that Fourier components of the envelope function lie well inside the first Brillouin zone). For a superlattice, this is written as

$$\psi(\mathbf{r}) = e^{iqz} \sum_j^{\Gamma} f_j(z) \chi_j(x,y) |u_{jT}(\mathbf{r})\rangle, \quad (2.17)$$

which must be compared with Eq. (2.6). The general function $f(\mathbf{r})$ has been separated into an envelope function $f(z)$ in the growth direction and an as-yet unspecified function $\chi(x,y)$ modulating the wave function in the plane of the layers (the e^{iqz} term is a result of the Bloch theorem for a superlattice potential, and so would be dropped for a heterojunction or quantum well. In the absence of applied fields, $\chi_j(x,y) = e^{ik_{\parallel}r}$ for all j). As in bulk, eigenstates of the structure will be a superposition of the Kane basis states. There is more involved in Eq. (2.17) than the envelope functions, however. It is implicitly assumed that the Kane basis states of Table 2.2 are identical in all heterostructure layers. This second, implicit assumption is perhaps the most drastic of the two. Calculations performed with different Kane basis states in each layer indicate that the assumption is valid for most material systems [5].

2.2.1.1 Bulk Hamiltonians in Arbitrary Growth Directions

Calculating the electronic structure of the heterostructure using the EFA requires a substitution analogous to the $k \cdot p$ method described earlier. That is, the form of the wave function needs to be substituted back into the SWE, to obtain a solvable expression for the envelope functions. In practice this involves using the bulk Hamiltonian matrices, considering the band offsets between materials and the band-edge potential.

However, I have used two separate definitions of the z -direction, and that needs to be addressed at this point. In the $k \cdot p$ case, the z -direction is a well-defined direction in the crystal lattice, determined by the orientation of the tetragonal chemical bonds between atoms. However, I have also defined z as the growth direction in the heterostructure. The two definitions of z will coincide *only* for structures grown in the [001] direction. Happily, the [001] direction is a popular growth direction, and so in most cases the bulk Hamiltonian matrix is acceptable as it stands.

However, there are often distinct advantages to growing in directions other than [001]. Non-[001] structures will have nonzero piezoelectric fields (assuming some lattice mismatch),

which may influence the electronic structure. Carrier effective-mass anisotropy might also make other orientations desirable, if different masses improve electrical or optical properties. For many of the samples studied experimentally in this thesis, the [111] growth direction was used. Crystals of zincblende symmetry cleave easily in the [111] plane, hence high-quality substrates are easy to obtain. Also, the piezoelectric field has a maximum in the [111] direction, and for the InAs/GaSb system the hole [111] effective masses are lighter than their [001] values.

Therefore, the case of heterostructures grown in non-[001] orientations needs to be considered. One would be tempted to directly rotate the [001] wave vector operators k_x , k_y , and k_z , to point in the new orientation. This fails, however, as the construction of the bulk Hamiltonians implicitly quantized the spin of the carriers in the [001] direction, for the treatment of spin-orbit splitting and spin splitting of states in a magnetic field to be valid. So a simple rotation of coordinates is not allowed. What is required is a rotation of the axis of quantization.

The procedure I have used for calculating a bulk Hamiltonian of arbitrary orientation is as follows [7]:

- 1) Rotate the k -vectors to the new coordinate basis.
- 2) Construct bulk atomic wave functions such that spin is quantized in the new coordinate basis.
- 3) Construct a Kane basis set such that the spin-orbit interaction is diagonalized.
- 4) Calculate the bulk Hamiltonian using this new Kane basis set.

In practice, all but the fourth step are very straightforward. To illustrate, I demonstrate the procedure for the [111] direction. First, the k -vectors are rotated to a new set, k_1 , k_2 , and k_3 . The k_3 vector is uniquely determined by the growth direction, k_2 is then chosen orthogonal to k_3 , and k_1 is determined as orthogonal to k_2 and k_3 . Thus for the [111] orientation:

$$\begin{aligned} k_1 &= \frac{1}{\sqrt{2}} (1, -1, 0), \\ k_2 &= \frac{1}{\sqrt{6}} (1, 1, -2), \\ k_3 &= \frac{1}{\sqrt{3}} (1, 1, 1). \end{aligned} \tag{2.18}$$

I then construct wave functions with spin quantized in the growth direction. The $|s\rangle$ wave function is completely isotropic, hence spin can be quantized in any direction. For the other three wave functions, the situation is directly analogous to the case of the wave vectors above. Just as the new k_i 's were constructed from the old k_i coordinates, so the new bulk wave functions are constructed from the old Bloch functions. For the [111] case, the wave functions are:

$$\begin{aligned}
|\Phi_s\rangle &= |s\rangle, \\
|\Phi_x\rangle &= \frac{1}{\sqrt{2}}(|x\rangle - |y\rangle), \\
|\Phi_y\rangle &= \frac{1}{\sqrt{6}}(|x\rangle + |y\rangle - 2|z\rangle), \\
|\Phi_z\rangle &= \frac{1}{\sqrt{3}}(|x\rangle + |y\rangle + |z\rangle),
\end{aligned} \tag{2.19}$$

where the $|\Phi_\alpha\rangle$ spin points along the α direction in the new coordinates.

Finally, a set of basis functions is constructed which diagonalizes the spin-orbit interaction, a set which for *all* orientations (given the appropriate $|\Phi_\alpha\rangle$ wave functions) has the form given in Table 2.3. It is clear that the [001] Kane Γ states listed in Table 2.2 are a special, simple case of the general states in Table 2.3.

With the basis states now constructed, one calculates the bulk Hamiltonian using Eq. (2.14) as before. This time, however, the bulk wave functions $|\Phi_i\rangle$ are themselves

Table 2.3: Generalized Γ -point basis functions.

	$ j, m_j\rangle$	Ψ_{jm}	E_Γ
c $\uparrow$	$ 1/2, +1/2\rangle$	$ \Phi_s\uparrow\rangle$	E_G
hh $\uparrow$	$ 3/2, +3/2\rangle$	$\frac{1}{\sqrt{2}}(i \Phi_x\uparrow\rangle + \Phi_y\uparrow\rangle)$	0
lh $\downarrow$	$ 3/2, -1/2\rangle$	$\frac{1}{\sqrt{6}}(i \Phi_x\uparrow\rangle - \Phi_y\uparrow\rangle - 2i \Phi_z\downarrow\rangle)$	0
so $\downarrow$	$ 1/2, -1/2\rangle$	$\frac{1}{\sqrt{3}}(i \Phi_x\uparrow\rangle - \Phi_y\uparrow\rangle + i \Phi_z\downarrow\rangle)$	$-\Delta$
c $\downarrow$	$ 1/2, -1/2\rangle$	$ \Phi_s\downarrow\rangle$	E_G
hh $\downarrow$	$ 3/2, -3/2\rangle$	$\frac{1}{\sqrt{2}}(i \Phi_x\downarrow\rangle - \Phi_y\downarrow\rangle)$	0
lh $\uparrow$	$ 3/2, +1/2\rangle$	$\frac{1}{\sqrt{6}}(i \Phi_x\downarrow\rangle + \Phi_y\downarrow\rangle + 2i \Phi_z\uparrow\rangle)$	0
so $\uparrow$	$ 1/2, +1/2\rangle$	$\frac{1}{\sqrt{3}}(i \Phi_x\downarrow\rangle + \Phi_y\downarrow\rangle - i \Phi_z\uparrow\rangle)$	$-\Delta$

superpositions of s and p states, hence the algebra is an order of magnitude more tedious. Again, however, a computer can solve the problem quickly and accurately. The [111] bulk Hamiltonian matrix calculated in this way is presented in Appendix A. Although the intermediate steps are more complicated, the [111] direction is symmetric enough to lead to a Hamiltonian only marginally more complicated than the [001] case.

The algorithm for generating bulk Hamiltonians in arbitrary growth directions is fairly straightforward, and one therefore has the capability to perform EFA modeling of heterostructures of any growth orientation. In the following discussion of EFA techniques, I shall adopt convention and refer to z as the growth direction, although it is understood that this is often not the same z as the crystal lattice.

2.2.1.2 Block-Diagonalization of the Hamiltonian

Without an applied field, the eight basis states are spin-degenerate. Cohen *et al.* [8] have shown that in this case there exists a unitary transformation

$$U = \begin{pmatrix} R & R \\ R^* & -R^* \end{pmatrix}, \quad (2.20)$$

such that

$$U^\dagger H U = \begin{pmatrix} H_D & 0 \\ 0 & H_D^* \end{pmatrix}, \quad (2.21)$$

where R is a diagonal 4x4 matrix, and H_D is the block-diagonalized 4x4 Hamiltonian containing four non-degenerate states. The form of the unitary transformation in Eq. (2.20) assumes that the basis set is ordered as in Table 2.3. The transformation of Eq. (2.21) only block-diagonalizes certain terms in the Hamiltonian, however. In particular, terms containing the “warping” parameter $\mu \propto (\gamma_2 - \gamma_3)$ present a problem, and Cohen *et al.* avoid this by including the non-block-diagonalized terms as a perturbation. I set $\mu = 0$ as a convenient simplification (known as the axial approximation). This is not the same as setting $\gamma_2 = \gamma_3$ (the spherical approximation), as μ is set to zero only in the four off-diagonal terms where it appears. The axial approximation thus keeps much of the anisotropy of the in-plane

dispersion, yet still allows for the convenient block-diagonalization of the bulk Hamiltonian [9,10].

Much of the matrix manipulations required by the EFA are of order n^3 , where n is the dimension of the Hamiltonian. Hence a reduction of the size of the matrices results in a significant increase in calculation speed. Although the Hamiltonian cannot be block-diagonalized in this manner for an applied magnetic field (because the transformation of Eq. (2.21) requires that k_x and k_y commute), the axial approximation results in an important simplification in the form of the wave function, which again increases the speed of computation without sacrificing much accuracy.

2.2.1.3 Form of the Hamiltonian and Interface Boundary Conditions

The bulk Hamiltonian matrix of Eq. (2.14), constructed with the basis of Table 2.3, is separated into coefficients of the growth-direction momentum operator k_z . A Hermitian form for these coefficients must be chosen, although there is no unique Hermitian formulation [11]. I use the common form

$$H\psi = [k_z H_2 k_z + \frac{1}{2} (H_1 k_z + k_z H_1) + H_0] \psi = E\psi. \quad (2.22)$$

The boundary conditions are determined uniquely from the form of the Hamiltonian, and the requirement that the wave function ψ is continuous everywhere. One integrates the wave function operated upon by the Hamiltonian across an interface at $z = 0$,

$$\lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{\varepsilon} H\psi dz = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{\varepsilon} E\psi dz = 0, \quad (2.23)$$

which for the form of Eq. (2.22) requires that the quantity

$$H_2\psi' + \frac{i}{2} H_1\psi \quad (2.24)$$

be constant across an interface. Eq. (2.24), plus the continuity of the wave function, is then the boundary condition to be obeyed at an interface. In a heterostructure, valid envelope

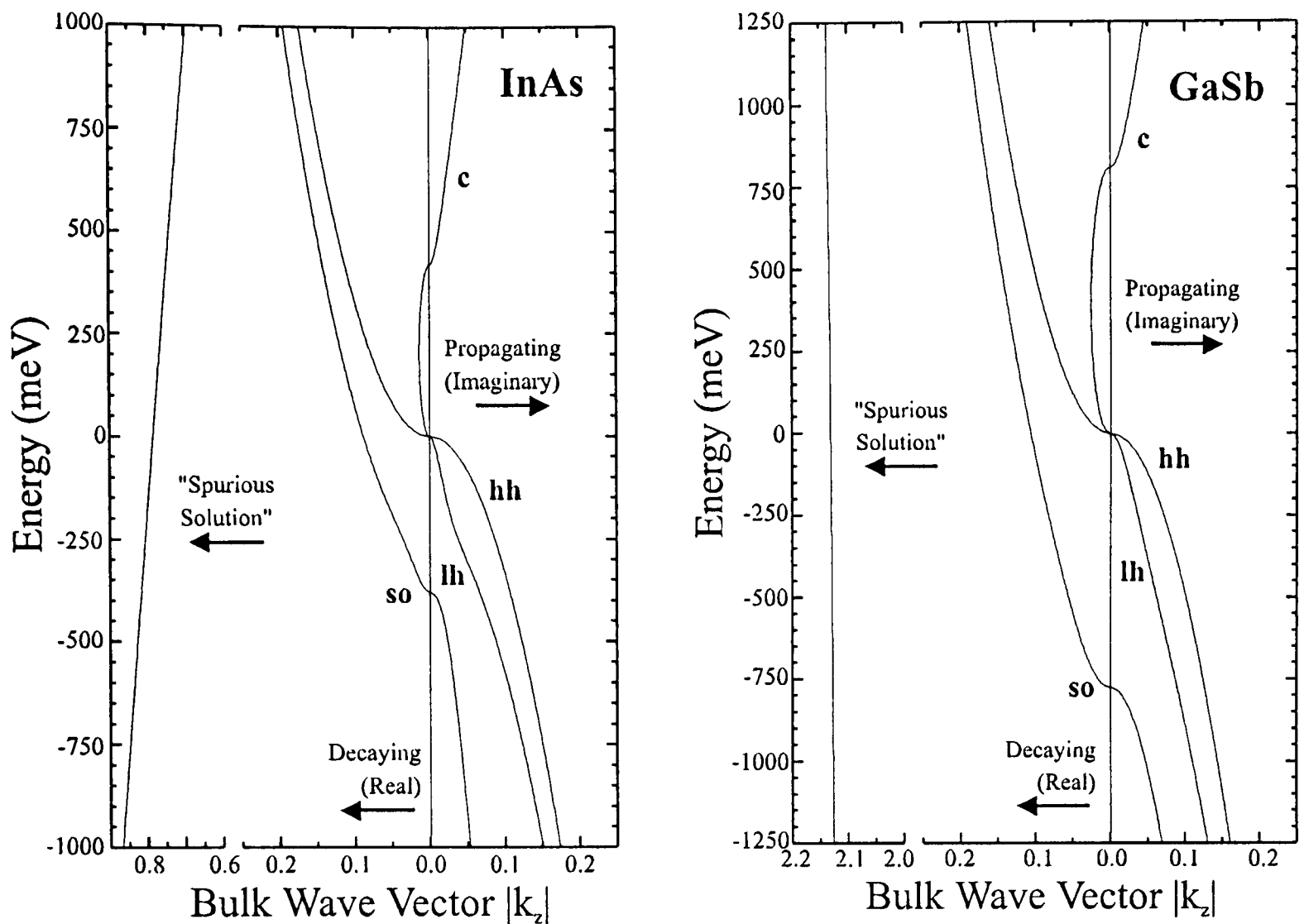


Figure 2.4: Bulk k_z dispersions for InAs and GaSb, calculated for $k_{\parallel} = 0$ using the transfer-matrix method (described below). Each line is doubly-degenerate (momentum in the + and - z-direction), quadruply degenerate if spin degeneracy is included. In the Ram-Mohan model, real k_z corresponds to decaying solutions under the barrier, while imaginary solutions propagate. Note the large decaying solutions for each material: these are the “spurious solutions” which cause problems with transfer-matrix methods.

functions are solutions of the Hamiltonian of Eq. (2.22) which satisfy the boundary conditions of Eq. (2.24).

The outline of the EFA method is as follows: with the wave function in the form of Eq (2.17), within each layer of the heterostructure it is assumed that the wave function propagates as it would through bulk. A trial SL bound state energy is selected, then either explicitly or implicitly one calculates the k_z (growth direction bulk momentum wave vector) of the electron as a function of its momentum in the layer planes and energy relative to the bulk band gap within each layer. States far away from the band gap will have a large k_z , while states close in energy to the gap will have small k_z values. States actually inside the band gap (which can occur for heterostructures), will have imaginary k_z values. The k_z dispersions for InAs and GaSb are shown in Fig. 2.4. The wave function boundary conditions are then used to determine whether the trial energy is a valid bound state of the heterostructure, and so the electronic structure is calculated. (The large, unphysical k_z values in each material are referred

to as “spurious solutions,” and arise from coupling between the valence and conduction bands. They are a major obstacle to EFA modeling, of which more will be said later.)

The first method I describe, the transfer-matrix technique, follows the above outline almost to the letter, and so is a very clear algorithm. Unfortunately, it suffers from several drawbacks, mostly due to the spurious solutions. The second method, the “momentum-matrix” technique, works in momentum space instead of real space, and so is (for those versed in transfer-matrix techniques) less intuitive. Nonetheless, it is much more powerful, and is the backbone of real device modeling presented later in the thesis.

2.2.2 The Transfer-Matrix Technique

The most popular method of calculating the electronic structure of heterostructures within the envelope-function approximation is the transfer-matrix technique. The name derives from the fact that for each layer, a matrix is constructed representing the propagation of the multi-component wave function (similar to how one calculates the propagation of light waves through material layers of different refractive indices). One solves for the wave function at a particular point, and then uses the transfer matrices to find the wave function at other points in the structure. The actual construction of the transfer matrices involves the bulk Hamiltonian matrices and appropriate boundary conditions at the heterostructure interfaces.

2.2.2.1 General Multi-Band Models

Ram-Mohan *et al.* [12] have given a compact algorithmic treatment of the transfer-matrix method, which allows for an intuitive picture of the process, as well as pointing out the limits of the method. Although it differs in form from other transfer-matrix techniques, the underlying physics is the same. The majority of the analysis of semiconducting samples presented in Chapter 6 was performed using this Ram-Mohan method.

One begins with the boundary conditions. A vector f of twice the dimension of the Hamiltonian is defined with components

$$f = \begin{pmatrix} \psi \\ H_2 \psi' + \frac{i}{2} H_1 \psi \end{pmatrix}. \quad (2.25)$$

With this definition of f , the boundary conditions on the wave function are automatically satisfied by requiring that f be continuous everywhere. The derivative of f is then taken, and the SWE of Eq. (2.22) is used to eliminate the second differentials of ψ . What results is a set of coupled linear differential equations for f of the form

$$\frac{\partial}{\partial z} f = \Lambda f, \quad (2.26)$$

where Λ is a matrix with elements

$$\Lambda = \begin{pmatrix} -\frac{i}{2} H_1 H_2^{-1} & H_2^{-1} \\ (H_0 - E) - \frac{1}{4} H_1 H_2^{-1} H_1 & -\frac{i}{2} H_2^{-1} H_1 \end{pmatrix}. \quad (2.27)$$

It is at this point that the first limitation of the transfer-matrix approach is encountered. Eq. (2.26) can *only* be solved in the case where $\Lambda(z_1)$ commutes with $\Lambda(z_2)$ for all z_1 and z_2 . In practice, given the form of Λ in Eq. (2.27), this means that Eq. (2.26) can only be solved when all Hamiltonian coefficient matrices H_i are constant. Within each layer, therefore, the band-edge potential must be flat.

If Λ is constant, then Eq. (2.26) is solved analogous to the one-dimensional linear differential equation $y' = my$ to find

$$f(z) = \exp(\Lambda z) f(0). \quad (2.28)$$

The exponential of the matrix Λz is given by

$$\exp(\Lambda z) = P^{-1} \exp(\lambda z) P, \quad (2.29)$$

where λ and P are the eigenvalues and eigenvectors, respectively, of the Λ matrix. Eq. (2.29) is a very reliable method of obtaining exponentials, even for general complex matrices with degenerate eigenvalues, so long as the eigenvectors P are constructed to be orthogonal.

To find the bound states within a superlattice, the propagation of the wave function is tracked across a superlattice period. I use two layers in the equations below, but the method can obviously be extended to apply to any number of layers per superlattice period.

For a two-layer structure, the vector $f(d)$ is described by the propagation of f across both layers via Eq. (2.28), and so produces an expression defining the superlattice transfer-matrix M :

$$f(d) = \exp(\Lambda_B l_B) \exp(\Lambda_A l_A) f(0) = M f(0), \quad (2.30)$$

where l_i and Λ_i are the thickness and Λ matrix for layer i , and $d = l_A + l_B$ is the superlattice period. The Bloch condition

$$f(d) = e^{iqd} f(0), \quad (2.31)$$

is applied to arrive at the superlattice determinantal equation

$$M f(0) = e^{iqd} f(0). \quad (2.32)$$

To find the electronic structure for a given in-plane momentum and q point, one scans in energy until Eq. (2.32) is satisfied, that is, until the matrix M has an eigenvalue e^{iqd} . The eigenvector corresponding to e^{iqd} is then $f(0)$, and f may be determined at any other point in the structure through use of Eq. (2.28). The band structure of sample 1698, as calculated by the Ram-Mohan technique, is presented in Fig. 2.5.

Although the theory requires that the band-edge potential be constant, arbitrary potentials can be accommodated by breaking the layers up into small sections, where the potential is considered to be constant in each one. This mesh technique fails in practice, however, due to the problem of spurious solutions.

In Fig. 2.4, the phenomenon of spurious k_z solutions first appeared. They are wave vectors existing well outside of the first Brillouin zone, and they occur in any system where conduction and valence band coupling is included. If the spurious solutions are imaginary, that is, they correspond to propagating solutions, then they lead to spurious energy solutions of Eq. (2.32). If the spurious solutions are real, and so correspond to decaying states, then

they do not lead to spurious energy solutions, but cause numerical headaches when dealing with the exponentials in Eq. (2.29).

Unfortunately, the spurious solutions cannot simply be dropped. Although they correspond to unphysical states, they influence the physical states of the structure. The most common technique for dealing with spurious solutions is to include a cut-off wave vector k_c , of the order $k_c \approx 0.1 - 0.3 \text{ \AA}^{-1}$, such that any wave vector $|k_z| > k_c$ is truncated

$$k_z' = k_c \frac{k_z}{|k_z|}. \quad (2.33)$$

The truncation wave vector k_c is then varied. If any eigenstates E of Eq. (2.32) are sensitive to k_c , they are assumed spurious, and so are ignored. Likewise, the introduction of a cut-off helps to control the numerical problems of exponentiating large numbers.

Unfortunately, truncation is not a sure fix. If a large number of layers are included (for instance, when trying to solve for an arbitrary potential), then the spurious solutions dominate the exponential terms, and physical wave vectors are lost due to the finite numerical precision

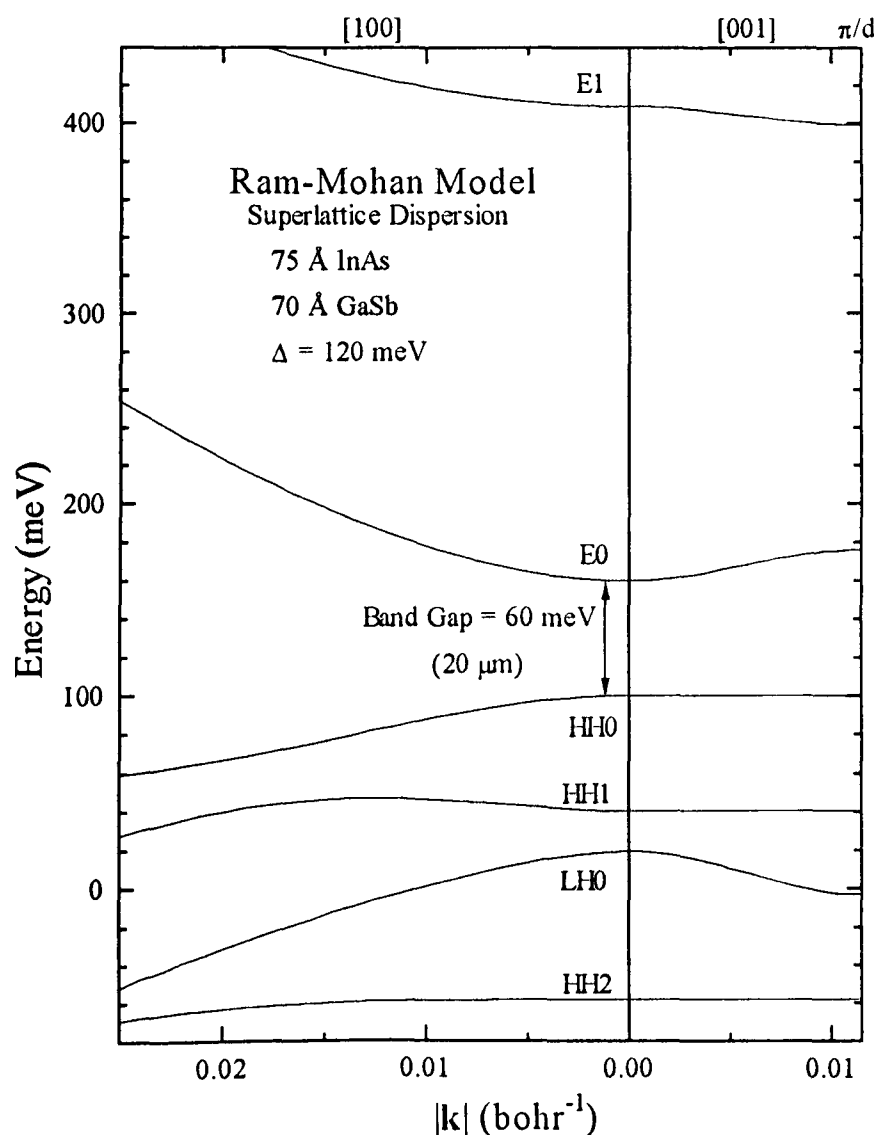


Figure 2.5: Band structure of sample 1698 as calculated from the Ram-Mohan transfer-matrix method.

of the computer. Likewise, even for only a few layers, large layer thicknesses result in problems when exponentiating, and so accurate solutions to Eq. (2.32) cannot be found until even the physical k_z solutions are truncated.

Smith and Mailhot [7] avoid the problem of spurious solutions by dropping some curvature terms along the diagonal of the Hamiltonian. The resulting EFA method is more complicated, but spurious solutions do not arise, even with conduction and valence band coupling. Their justification for dropping the curvature

terms is that much of the curvature of bands comes from off-diagonal coupling terms. However, the Smith and Mailhot method also requires flat-band conditions, and so heterostructures of arbitrary potential profile must be broken into a fine mesh of layers.

Transfer-matrix techniques, then, are suited only for thin-layer structures, with flat or nearly-flat band-edge potentials. They are popular due to their relative ease of computation, and to the physical intuition that arises from working in real space. For much of the work done here with InAs/GaSb heterostructures, however, the crossed-gap nature of the system leads to significant charge transfer and so large band-bending. Therefore an alternative to the transfer-matrix method is desired.

2.2.2.2 *Single-Band Models (Effective Mass Method)*

For large band gap systems (e.g., GaAs/AlGaAs), the conduction-valence band coupling is small, and can be neglected to first order. In this case, one assumes that conduction band subbands are pure spin-degenerate $|s\rangle$ states. The transfer-matrix method is then much simpler to construct. The Hamiltonian of Eq. (2.14) can be represented in a single, one-dimensional wave equation for the envelope function $f(z)$ modulating the $|s\rangle$ Kane basis state:

$$\left(-\frac{1}{2m^*} \frac{\partial^2}{\partial z^2} + \frac{k_{\parallel}^2}{2m^*} + V(z) \right) f = E f, \quad (2.34)$$

where $k_{\parallel}$ is the wave vector in the plane of the layers. All of the influences of farther bands are neatly tucked into a single parameter m^* , the “effective mass” of the electron in the conduction band. For systems with large band gaps (weak coupling with the valence band), m^* will be large ($m^* = 0.0665 m_0$ for GaAs), while small band gap systems will have smaller masses ($m^* = 0.023 m_0$ for InAs, $m^* \leq 0.01 m_0$ for near-zero band gap systems such as $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$).

For most III-V semiconductors, the valence band is the closest set of bands in energy to the conduction band, and therefore accounts for most of the coupling in the Löwdin perturbation. As an electron in the conduction band moves to higher energy states (either higher subbands, or higher $k_{\parallel}$ values), coupling with the valence band will weaken (since Löwdin perturbation terms scale inversely with the energy separation of the bands), and the effective mass m^* will get heavier, approaching the free electron mass. This is the

phenomenon of nonparabolicity, which can be measured experimentally. Again, nonparabolicity is most pronounced in small band gap systems, as even small changes in energy can correspond to a large proportion of the band gap energy.

For the case of an arbitrary potential $V(z)$, Eq. (2.34) can be solved numerically. This is the real advantage of the effective-mass technique. The heterostructure is broken into a mesh of finely-spaced points along the growth direction z , and the SWE of Eq. (2.34) is transformed into a divided-difference equation, using the simple Euler formulas

$$\begin{aligned} y(z)' = \frac{\partial}{\partial z} y &\rightarrow y_i' = \frac{y_{i+1} - y_{i-1}}{2h}, \\ y(z)'' = \frac{\partial^2}{\partial z^2} y &\rightarrow y_i'' = \frac{y_{i+1} + y_{i-1} - 2y_i}{h^2}. \end{aligned} \quad (2.35)$$

Eq. (2.35) assumes a constant mesh spacing h between points, although the equations can be generalized for arbitrary mesh spacings. Likewise, the accuracy of the divided difference equations can be improved by more sophisticated techniques, such as Runge-Kutta [13,14]. Nonetheless, Eq. (2.35) is accurate to second order in h , which is sufficient for accurate solutions given a fine enough mesh spacing.

Using the divided-difference expressions of Eq. (2.35), the SWE of Eq. (2.34) gives an expression relating the envelope function at adjacent mesh points:

$$f_{i+1} = \{ 2 + h^2 [k_{||}^2 + 2m^* (V_i - E)] \} f_i - f_{i-1}. \quad (2.36)$$

To construct a wave function, two initial points f_0 and f_l are assumed, and then Eq. (2.36) is applied repeatedly to determine f_i at consecutive points i in the heterostructure mesh. For most energies, application of Eq. (2.36) will result in unphysical envelope functions. As with the multi-band transfer-matrix methods above, one scans in energy and uses the heterostructure boundary conditions to find the bound states of the system. The boundary conditions used are:

<i>Heterostructure</i>	<i>Boundary Condition</i>	
<i>Quantum Well, Heterojunction</i>	$f_N = 0$	(2.37)
<i>Superlattice</i>	$f_N = e^{iqd} f_0$	

where N is the final mesh point in the heterostructure.

In Eqs. (2.34) and (2.36), it is obvious that the $k_{||}$ term affects only the energy of the system, and not the wave functions themselves. Therefore, one can solve for the subband wave functions of the system just at $k_{||} = 0$, since $f(k_{||}, z) = f(0, z)$.

One can make similar assumptions about the valence band states. Wave equations for the heavy holes and light holes are constructed in a similar manner to Eq. (2.34), using effective masses m_{hh}^* and m_{lh}^* respectively. Heavy hole states are assumed to be pure $|^{3/2}, \pm^{3/2}\rangle$, and light holes pure $|^{3/2}, \pm^{1/2}\rangle$. Here the assumption has no physical justification, since valence states mix strongly for finite $k_{||}$ (or finite magnetic field). Nonetheless, solving for valence states using the effective mass approximation is much faster than solving a real multi-band Hamiltonian. And the concept of effective mass still holds for the valence band, where experimentally observed valence band transitions can be assigned effective masses in the same way as conduction band transitions.

Solving InAs/GaSb heterostructures using the effective mass approximation leads to inaccurate subband energies, and fails to account for the mixing between basis states. However, the method leads to remarkably accurate predictions of carrier densities for a wide range of heterojunction and superlattice thicknesses [13,19]. Given the partial success of the effective mass approximation in describing InAs/GaSb systems, and its near-total success describing large band gap type-I systems [11], one can see that the approximations involved hold for a wide range of materials.

2.2.3 The “Momentum-Matrix” Technique

For all of the advantages of the effective mass approximation (EMA), however, its lack of band mixing eventually leads to problems when modeling the crossed-gap InAs/GaSb system. For semiconducting superlattices, where the EMA might be expected to be most accurate, the observed superlattice band gaps cannot be reproduced without applying unphysical effective masses (as in Chapter 6, and ref. [20]). Likewise, for semimetallic superlattices, although the EMA correctly predicts the total carrier density, it consistently fails

to predict the correct number of populated subbands [21]. And for both semiconducting and semimetallic superlattices, the EMA completely fails to predict some observed valence band transitions [19, 20]. Band mixing must therefore be included in modeling. However, as shown above, the transfer-matrix technique cannot handle arbitrary band-edge potentials, or large layer thicknesses. For semimetallic InAs/GaSb structures, a model is needed which can handle both.

The solution I present is the “momentum matrix” technique, so-called because whereas the transfer-matrix technique constructs matrices representing the physical propagation of the wave function in real space, this method constructs a matrix representing the evolution of the wave function in momentum space. The model contains the basic elements of pseudopotential techniques [6] and can also be thought of as an extension of the work of Winkler and Rössler [15] to superlattices, although it is essentially the decades-old solution of the wave equation of an electron in a periodic potential [22]. In addition to being flexible with respect to band-edge potentials and layer thicknesses, the method is also algorithmically compact, being fully described by only a few equations.

The forms of the wave function ψ and the Hamiltonian H are those given by Eqs. (2.17) and (2.22), respectively. Instead of turning to real space to determine the propagation of the wave function through each layer, the periodicity of the superlattice is exploited. The potential has the property $V(z+d) = V(z)$, as do the Hamiltonian and envelope functions (with the notable exception of the e^{iqz} term). A Fourier expansion of those functions will therefore contain only harmonics of the reciprocal superlattice wave vector, $2\pi/d$. Analogous to the case of the pseudopotential technique [6], a set of reciprocal superlattice vectors is defined with elements $G_n = 2\pi n/d$. The Hamiltonian matrices, potential, and envelope functions are then expanded in terms of these reciprocal superlattice vectors:

$$\begin{aligned} H_i(z) &= \sum_n T_{i,n} e^{iG_n z}, \\ V(z) &= \sum_n V_n e^{iG_n z}, \\ f(z) &= \sum_n f_n e^{iG_n z}. \end{aligned} \tag{2.38}$$

These expressions are substituted back into the SWE of Eq. (2.22), resulting in an expression relating the Fourier coefficients of the Hamiltonian, potential, and envelope function:

$$\sum_m [(q+G_n)(q+G_m)T_{2,n-m} + (q + \frac{1}{2}(G_n + G_m))T_{1,n-m} + T_{0,n-m} + V_{n-m}] f_m = E f_n \quad (2.39)$$

This can be re-written as a matrix eigenvalue equation

$$M(q) F = E F, \quad (2.40)$$

where the elements of eigenvector F are the Fourier coefficients of the envelope function f_n , and the matrix $M(q)$ is defined

$$M_{ij}(q) = (q + G_i)(q + G_j)T_{2,i-j} + (q + \frac{1}{2}(G_i + G_j))T_{1,i-j} + T_{0,i-j} + V_{i-j}. \quad (2.41)$$

To find the electronic structure of the superlattice at a given $k_{\parallel}$ and q , one constructs the $M(q)$ matrix and diagonalizes it. The eigenvalues of the matrix are the eigenenergies, and the corresponding eigenvectors are the Fourier coefficients of the envelope function. Sample 1698 has been solved using the momentum-matrix method, as it was for the transfer-matrix method, and the result is plotted in Fig 2.6. In this case I was able to include the effects of alternate interface types (to be discussed in later chapters), which leads to a “tilting” of the band-edges. The bands are very similar to those calculated with the transfer-matrix technique (Fig. 2.5), as one would expect.

Mention should be made of the computing requirements of the momentum-matrix method.

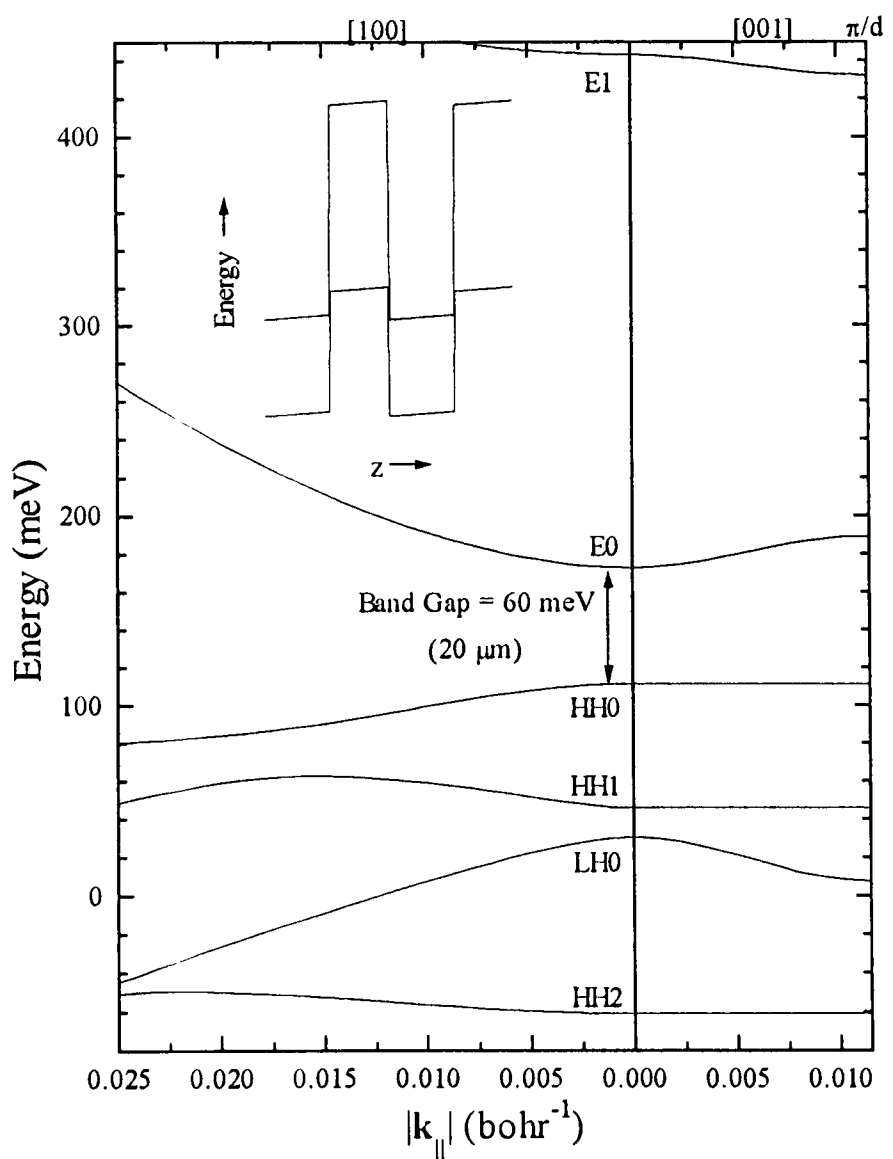


Figure 2.6: Band structure of sample 1698, as calculated from the momentum-matrix technique. The layer thicknesses are as in Fig. 2.5. The band-edge potential is inset.

elements $M_{ij}(q)$ in Eq. (2.41) are themselves matrices, of the dimension of the Hamiltonian. The total dimension of the $M(q)$ matrix will be the dimension of the Hamiltonian, multiplied by the number of terms in the Fourier expansion, usually on the order of twenty or thirty. So for 8-band Hamiltonians, the $M(q)$ matrix could be as large as 240x240. Although this is much larger than standard transfer-matrix approaches with matrices only double the size of the Hamiltonian, it must be pointed out that in transfer-matrix approaches, the total transfer-matrix of the superlattice must be calculated at a large number of energy steps, where a root-hunting algorithm is used to find bound states to an acceptable tolerance. A calculation of several electronic states at a given $(q, k_{\parallel})$ value may require literally hundreds of evaluations of the superlattice transfer-matrix. In the momentum-matrix method, the $M(q)$ matrix is calculated only once per $(q, k_{\parallel})$ point, with the eigenenergies of the system determined by a diagonalization procedure. The accuracy of the eigenvalues is determined solely by the number of Fourier terms included (as most matrix eigenvalue routines are accurate to far better than 1 in 10^8). For semiconducting superlattices, where fewer Fourier terms are required (since one is typically only interested in states near the band gap), I find the momentum-matrix method to be as fast or faster than the transfer-matrix approach, with an increase in stability as well. Typical running times for semiconducting superlattices are on the order of a few minutes, on a DEC Alpha computer. For long-period superlattices, more Fourier terms are required to model the bands accurately, and this can require an hour or more of CPU time. A direct comparison with the transfer-matrix method is not possible in this case, however, as the spurious solutions render the problem intractable.

Most importantly, the momentum-matrix technique can handle arbitrary potentials and large layer thicknesses. The spurious k_z solutions are not a problem, since the Fourier series is truncated well before the Brillouin zone boundary, a truncation which only affects eigenstates far away from the superlattice band gap. The method is also very stable, due to the lack of root-hunting. Nearly-degenerate states can cause problems with transfer-matrix methods, but are easily handled by the momentum-matrix approach. This is important, since in semimetallic systems the eigenstates can be clustered very close together in energy. Finally, the momentum-matrix technique allows for modeling of more sophisticated superlattice structures, such as layers with graded composition, or complex doping profiles.

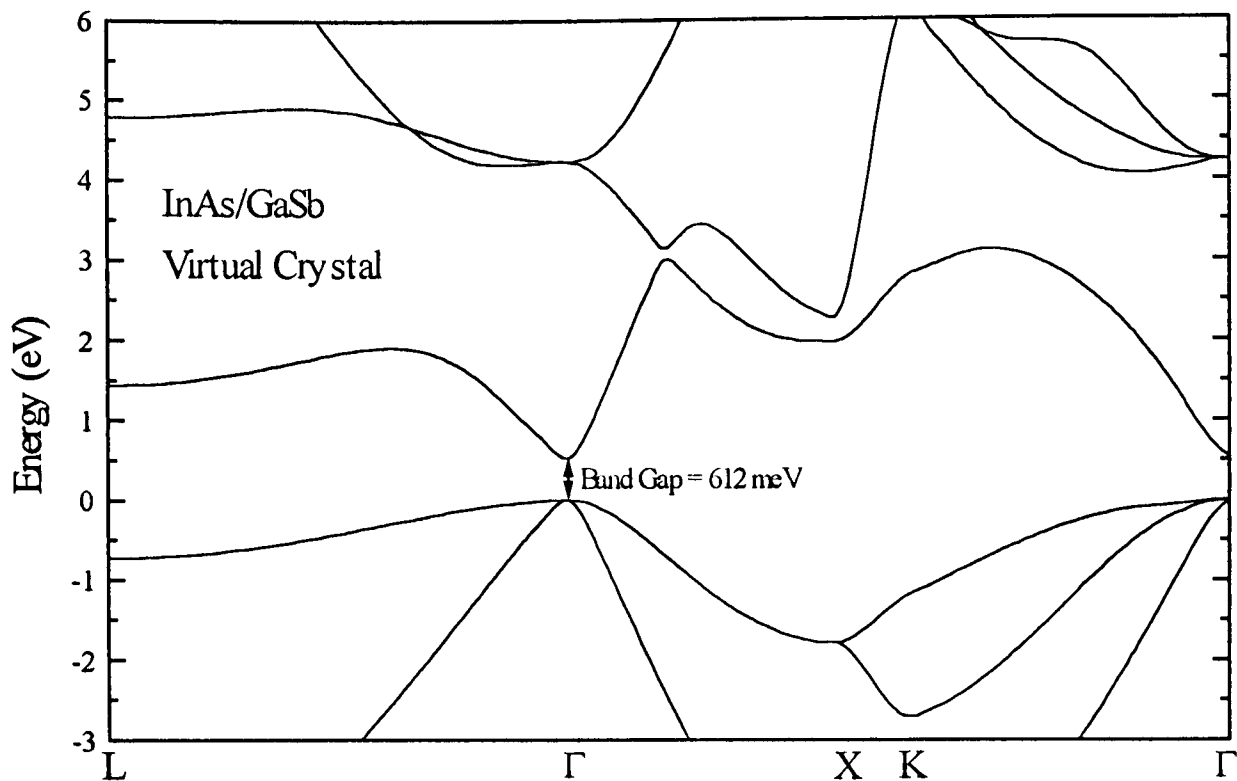


Figure 2.7: The band structure of an InAs/GaSb virtual crystal. The lattice constant and pseudopotential form factors of the crystal are taken to be an average of those of InAs and GaSb (ref. [7]).

2.2.4 Choice of a Basis Set

The assumption in Eq. (2.17), that the Kane basis states in all layers are equal, is a weak one, particularly in the InAs/GaSb system. Since the two materials have no elements in common, one would suspect that the Bloch functions in each material are likely to be somewhat different, a similar lattice constant notwithstanding. The fact that each material has a different Kane matrix element [24] bears out this view. Smith and Mailhot [7] and Burt [23] have both presented methods of dealing with this problem. Smith and Mailhot use the pseudopotential method to construct a “virtual crystal,” a crystal with a lattice constant and energy splittings which is taken to be an average of the heterostructure materials. They solve Eq. (2.5) at the Γ -point in the virtual crystal, and use those states as a basis for the EFA wave function. Burt, likewise, simply assumes plane waves as a basis.

With either technique, once a common basis is chosen, extra terms are added to the bulk Hamiltonian to account for the different Bloch functions in each layer. I attempted the virtual crystal approximation for the InAs/GaSb system using the transfer-matrix approach, but found that the method still had problems with wide layer thicknesses and spurious solutions, and was significantly more complicated by the compensating Bloch terms. Nonetheless, the use of a common basis in each layer has been shown to solve the problem of “arbitrary” envelope function boundary conditions [23], and so would be a useful extension to the momentum-matrix technique.

2.3 Application of Magnetic Field

With an applied magnetic field, the $\mathbf{P} = \mathbf{p} + \mathbf{A}$ operators can no longer simply be replaced by their expectation values $\mathbf{k}$. In the bulk case, one can still solve for the energy levels of the system regardless of field direction: one rotates the Hamiltonian to align the coordinates with the field direction (in exactly the same way as the Hamiltonian was rotated to align with the growth direction), and then the problem can be treated as carriers bound in the plane perpendicular to the field direction, with free dispersion in the field direction [1,2].

In a heterostructure, however, the coordinate choice is determined by the growth direction. Applying a field in any direction other than the growth direction results in very complicated momentum operators, which have to account for the mixed quantization effects of the heterostructure potential and the applied field.

If the field is in the growth direction, however, the situation can be described very simply. The magnetic field introduces a parabolic potential in the plane of the layers, hence our $\chi_n(x,y)$ functions from Eq. (2.17) are the well-known harmonic oscillator wave functions. The growth direction momentum operator k_z is untouched, and the in-plane momentum operators can be expressed in terms of the ladder raising and lowering operators by [25]

$$\begin{aligned} P_x &= \sqrt{\frac{B}{2}} (a + a^\dagger), \\ P_y &= i \sqrt{\frac{B}{2}} (a - a^\dagger), \end{aligned} \tag{2.42}$$

where the ladder operators have the property

$$\begin{aligned} a \chi_n &= \sqrt{n} \chi_{n-1}, \\ a^\dagger \chi_n &= \sqrt{n+1} \chi_{n+1}. \end{aligned} \tag{2.43}$$

With the axial approximation (discussed when block-diagonalizing the Hamiltonian, where the “warping” term $\mu \propto (\gamma_2 - \gamma_3)$ is set to zero in terms where it appears), the wave functions have the particularly simple form

$$\psi(\mathbf{r}) = e^{iqz} \sum_j^{\Gamma} f_j(z) \chi_{m(n,j)}(x,y) |u_{j\Gamma}(\mathbf{r})\rangle, \quad (2.44)$$

where only one $\chi_m(x,y)$ term is required in the expansion of each component of $\psi(\mathbf{r})$, and n is a quantum number. The dependence of m on n and j can be calculated in a straightforward way by operating on $\psi(\mathbf{r})$ by the Hamiltonian of Eq. (2.14), and is given in the Appendix.

To construct bulk Hamiltonians which account for a field in the growth direction, one replaces the operators P_x and P_y in the zero-field Hamiltonian matrix by their expressions in Eq. (2.42), and operates on the wave function of Eq. (2.44). This results in a matrix similar to the zero-field bulk Hamiltonian matrix, where the k_x and k_y wave vectors are replaced by functions

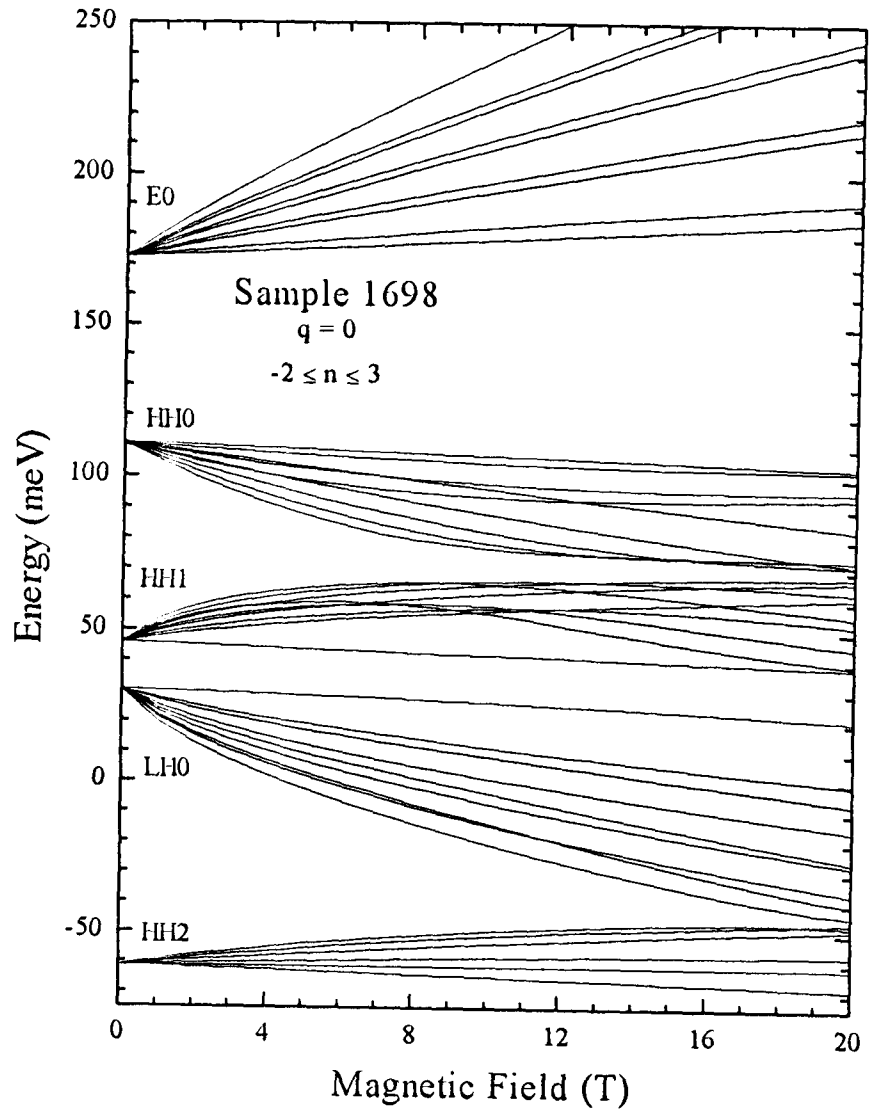


Figure 2.8: The magnetic field dispersion of sample 1698 (75 Å InAs, 70 Å GaSb), at $q=0$, for the first few Landau indices. Calculated by the momentum-matrix technique (see Fig. 2.6).

of n , and the field introduces spin-splitting along the diagonal. Magnetic field Hamiltonian matrices are presented in the Appendix, for the [001] and [111] directions. The magnetic field dispersion of sample 1698 has been calculated in this manner using the momentum-matrix technique, and is presented in Fig. 2.8.

The extra degree of quantization provided by a magnetic field applied in the growth direction is evident in Fig. 2.8. Just as a heterostructure potential splits the bulk bands into an infinite number of subbands, so the magnetic field splits each heterostructure subband into an infinite number of Landau levels.

2.4 Observables: Transitions and Selection Rules

In the previous three sections, I have outlined how to calculate the electronic structure of both bulk materials and heterostructures, with and without applied magnetic field. As experimentalists, however, we cannot directly probe the energy states and wave functions. We are instead concerned with observables, which for the purposes of this thesis means optical transitions between quantum states.

The exact nature of the transitions will depend on several external variables, most notably whether or not a magnetic field is applied, and if so in what direction. For the following discussion, I shall deal with general eigensolutions, and show how to derive transition selection rules for the specific cases which will arise in later chapters. I shall also only deal with heterostructure eigenstates.

Absorption processes are best illustrated by examining the equation for the absorption coefficient $\alpha(\omega)$ (in units of absorption per superlattice period per unit illuminated area) in the dipole approximation [26]

$$\alpha(\omega) = A \sum_{i,f} | \langle i | \boldsymbol{\varepsilon} \cdot \mathbf{p} | f \rangle |^2 \delta(E_f - E_i - \omega) [f(E_i) - f(E_f)], \quad (2.45)$$

with

$$A = \frac{4 \pi^2}{n c \omega}, \quad (2.46)$$

where ω is the frequency and $\boldsymbol{\varepsilon}$ the polarization of the incident radiation, n is the index of refraction and c the speed of light, the summation is over initial and final states i and f respectively, and $f(E)$ is the Fermi filling factor of a state at energy E . It is important to note that the state labels i and f are *not* subband indices, but instead label all states available to carriers. So for the zero magnetic field case, this includes the $k_{\parallel}$ -dispersion of each subband, and for the magnetic field case, this includes all of the Landau level indices.

Within the summation, there are three terms which define the absorption process: the first term, the dipole matrix element $| \langle i | \boldsymbol{\varepsilon} \cdot \mathbf{p} | f \rangle |^2$, determines the strength of the transition from state i to f purely as a consequence of wave function overlap, and also results in momentum conservation; the second term ensures energy conservation but also gives rise to

the joint-density-of-states; and the third term allows transitions only from occupied to unoccupied states. I assume a low-temperature Fermi distribution, and so to account for the third term the summation is restricted to states i below the Fermi level, and states f above it.

It is the dipole matrix element which gives rise to selection rules, and is studied here for the case with and without magnetic field (the joint-density-of-states will be discussed in Chapter 7). Normally incident light will be either left- or right-circularly polarized (σ_L or σ_R), with polarization vector $\boldsymbol{\varepsilon}_{\pm} = \boldsymbol{\varepsilon}_x \pm i \boldsymbol{\varepsilon}_y$, $\boldsymbol{\varepsilon}_{+(-)}$ corresponding to σ_R (σ_L). With the form of the wave function in Eq. (2.17), the expression for the dipole matrix element becomes

$$\langle i | \boldsymbol{\varepsilon} \cdot \mathbf{p} | f \rangle = \sum_{m,n}^{\Gamma} \langle u_{m\Gamma}(\mathbf{r}) e^{iq_i z} f_{im} \chi_{im} | p_{\pm} | e^{iq_f z} f_{fn} \chi_{fn} u_{n\Gamma}(\mathbf{r}) \rangle, \quad (2.47)$$

which, assuming that f_{im} and χ_{im} are approximately constant across a unit cell of the crystal (a valid assumption for envelope functions), reduces to

$$\langle i | \boldsymbol{\varepsilon} \cdot \mathbf{p} | f \rangle = \sum_{m,n}^{\Gamma} \left(\int_{-\infty}^{\infty} e^{i(q_f - q_i)z} f_{im}^* f_{fn} dz \right) \left(\int \chi_{im}^* p_{\pm} \chi_{fn} d^2 r_{\parallel} \delta_{mn} + \int \chi_{im}^* \chi_{fn} d^2 r_{\parallel} P_{mn}^{\pm} \right). \quad (2.48)$$

The first integral term conserves momentum in the z -direction, as the integral vanishes unless $q_f = q_i$. In addition, it is seen that in all cases, the strength of absorption of normally incident light depends on the overlap of the z -direction envelope functions.

The second integral contains two terms, which illustrate the absorption process in a heterostructure. The first term, with a delta function constraining $m = n$, is intersubband absorption. The second term is interband absorption, the strength depending on the overlap of the χ_{ij} functions, and the interband momentum matrix element $P_{mn}^{\pm}$, which couples basis functions of appropriate angular momentum. For the 8x8 Hamiltonians given in the Appendix, the P^+ matrix element provides $c\uparrow-hh\uparrow$, $c\downarrow-lh\uparrow$, and $c\downarrow-so\uparrow$ coupling. The P^- matrix element provides $c\downarrow-hh\downarrow$, $c\uparrow-lh\downarrow$, and $c\uparrow-so\downarrow$ coupling.

2.4.1 Zero Magnetic Field

With no applied field, the $\chi_{ij}(x,y)$ functions are plane waves $e^{ik_{\parallel}r}$, so that the integrals of Eq. (2.48) reduce to the simple form

$$\langle i | \boldsymbol{\varepsilon} \cdot \mathbf{p} | f \rangle = \sum_{m,n}^{\Gamma} \left(\int_0^d f_{im}^* f_{fn} dz \right) P_{mn}^{\pm} \delta_{qf,qi} \delta_{k_{\parallel}^{(f)}, k_{\parallel}^{(i)}}. \quad (2.49)$$

The momentum conservation is contained in the Kronecker delta functions. For normally incident light in the absence of a magnetic field, only transitions of an interband character are allowed. In the InAs/GaSb system, intersubband transitions are possible, as even predominantly conduction-band states still mix heavily with hole states. In the GaAs/AlGaAs system, however, the conduction band states are almost pure $|s\rangle$ states, hence absorption occurs only at energies above the GaAs band gap.

2.4.2 Applied Magnetic Field

With a magnetic field in the growth direction, the $\chi_{ij}(x,y)$ functions are the harmonic oscillator wave functions. In this case the momentum matrix element has the form

$$\langle i | p_{\pm} | f \rangle = \sum_{m,n}^{\Gamma} \left(\int_0^d f_{im}^* f_{fn} dz \right) \left(\sqrt{2 \omega_{if} k} \delta_{j(f,n), j(i,m) \pm 1} \delta_{m,n} + P_{mn}^{\pm} \delta_{j(f,n), j(i,m)} \right) \delta_{qf,qi}, \quad (2.50)$$

where $j(i,m)$ is the Landau level index of the m^{th} basis component of the i^{th} bound state, and $k = \max(j(i,n), j(f,n))$. Again, momentum conservation is assured by the Kronecker delta functions, although this time the in-plane momentum information is contained in the form of the harmonic oscillator wave functions. Eq. (2.50) states that transitions are allowed between the j and $(j + 1)$ Landau levels of the same subband, or between the same Landau levels of different bands.

The important point of Eq. (2.50) is that unlike the zero-field case, normally incident light can be absorbed within a subband. For wide-layer InAs/GaSb superlattices where interband wave function overlap is expected to be small, the cyclotron resonance absorption dominates the absorption spectra, as the overlap integrals are set to unity.

2.4.3 Type-I versus Type-II Selection Rules

In the case of symmetric potentials (that is, where the potential is symmetric with respect to the center of all superlattice layers), the selection rules can be conveniently

Table 2.4: Interband selection rules for type-I and type-II superlattices ($k_{\parallel} = 0$).

Transition $E_n \leftrightarrow H_m$	k_z value	Type-I	Type-II
n and m same parity (both even, both odd)	0 (Γ) π/d	allowed allowed	allowed forbidden
n and m opposite parity (one even, one odd)	0 (Γ) π/d	forbidden forbidden	forbidden allowed

expressed in terms of the parity of the states involved in the transition. Even when strain or interface effects break the potential symmetry, the effect is usually a small perturbation on the overall symmetry, so that these symmetric selection rules are a useful guide for transitions in general superlattice potentials. Intriguing differences are found between type-I and type-II band lineups [26,27]. In both the applied- and zero-field cases, the selection rules involve the overlap of envelope functions

$$Z_{ifmn} = \int_0^d f_{im}^* f_{fn} dz . \quad (2.51)$$

Here, again, i and f refer to the initial and final state (subband indices), and m and n refer to the basis set (the Kane basis). In the case where $m = n$ (intersubband absorption), the selection rules are the same in both type-I and type-II systems: transitions are allowed only between states of opposite parity.

Interband transitions (where $m \neq n$) then involve the overlap of electron and hole envelope functions. Here the spatial separation of carriers leads to a difference in selection rules. In type-I systems, the selection rules depend only on the parity of the states. In type-II systems, the selection rules depend on both the parity of the states and the growth-direction momentum k_z . The general selection rules at the k_z extrema are listed in Table 2.4. Although the selection rules of general k_z values will be blurred in type-II systems, the density of states has strong maxima at the zone edges ($k_z = 0$ and π/d), therefore the zone-edge selection rules should indicate the strongest transitions.

2.4.4 Influences of Far Bands

The selection rules above were derived for the wave function of the form in Eq. (2.17), that is, simply expanded in terms of the Kane basis set. In fact, the physical wave function will

include mixing with far Γ states, as in Eq. (2.13). If one explicitly includes these terms, then extra transitions are allowed. In GaAs, for instance, there is strong intersubband absorption in the valence band, even at normal incidence, due to this mixing [16]. There is even speculation that the GaAs conduction band could absorb normally incident light, if the structure were engineered properly [28].

In the InAs/GaSb system, however, the influence of far bands are a small perturbation to the absorption processes already active in the system. Since I have mostly concerned myself with cyclotron and/or interband transitions, I have ignored far band mixing in these derivations.

2.5 Final Note

In this chapter, I have outlined how one can apply $k\cdot p$ theory to solve for the electronic structure of semiconductor heterostructures. In later chapters, I will describe how knowledge of the electronic structure is used to model observable properties, and so allow for the comparison of experiment and theory. In Chapter 7, I will show some of the predictive power of the theory.

It is worth noting a curious recursive property of $k\cdot p$ and EFA theory, a property which has promise as a method of calculating very complex structures in the future. When solving for bulk electronic structure using the pseudopotential method, a basis was chosen (simple plane waves), and then crystal eigenstates were derived as appropriate linear combinations of the basis states. I then turned to heterostructures, and used the crystal eigenstates as the basis, defining final heterostructure eigenstates as appropriate linear combinations of those basis states. There is no reason not to continue the process, that is, to use the heterostructure eigenstates as a basis for a further set of solutions [29]. This process in particular can be used to solve physically useful but theoretically difficult situations such as a heterostructure in arbitrary magnetic field. So it is no exaggeration to say that as a method of calculating electronic structure, $k\cdot p$ theory, with its EFA extension, has matured well over the past four decades, and has every prospect of lasting many more.

2.6 References

- [1] J. M. Luttinger and W. Kohn, Phys. Rev. **97** (1955) 869; J. M. Luttinger, Phys. Rev. **102** (1956) 1030.

- [2] C. R. Pidgeon and R. N. Brown, Phys. Rev. **146** (1966) 575.
- [3] E. O. Kane, in *Handbook on Semiconductors*, edited by T. S. Moss, North-Holland, 1982, page 193.
- [4] M. H. Weiler, in *Semiconductors and Semimetals*, vol. 16, edited by R. K. Willardson and A. C. Beer, Academic Press, 1981, page 119.
- [5] R. J. Warburton, *D.Phil. Thesis*, Clarendon Laboratory, Oxford, 1991.
- [6] M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141** (1966) 789.
- [7] D. L. Smith and C. Mailhot, Phys. Rev. **B 33** (1986) 8345; C. Mailhot and D. L. Smith, Phys. Rev. **B 35** (1987) 1242; D. L. Smith and C. Mailhot, Rev. Mod. Phys. **62** (1990) 173.
- [8] A. M. Cohen and G. E. Marques, Phys. Rev. **B 41** (1990) 10608.
- [9] N. O. Lipari and M. Altarelli, Phys. Rev. **B 15** (1977) 4883.
- [10] U. Ekenberg and M. Altarelli, Phys. Rev. **B 32** (1985) 3712.
- [11] R. A. Morrow and K. R. Brownstein, Phys. Rev. **B 30** (1984) 678.
- [12] L. R. Ram-Mohan, K. H. Yoo, and R. L. Aggarwal, Phys. Rev. **B 38** (1988) 6151.
- [13] D. Symons, *D.Phil. Thesis*, Clarendon Laboratory, Oxford, 1994.
- [14] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes: The Art of Scientific Computing*, Cambridge University Press, Cambridge, 1986.
- [15] R. Winkler and U. Rössler, Phys. Rev. **B 48** (1993) 8918.
- [16] F. Szmulowicz and G. J. Brown, Appl. Phys. Lett. **66** (1995) 1659.
- [17] F. Szmulowicz and M. O. Manasreh, C. E. Stutz, T. Vaughan, Phys. Rev. **B 50** (1994) 11618.
- [18] W. L. Bloss, J. Appl. Phys. **66** (1989) 3639.
- [19] M. Lakrimi, T. A. Vaughan, R. J. Nicholas, D. M. Symons, N. J. Mason, and P. J. Walker, Solid State Elect. **37** (1994) 1227.
- [20] T. A. Vaughan, M. Lakrimi, R. J. Nicholas, N. J. Mason, and P. J. Walker, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D.J. Lockwood, World Scientific 1995, page 1256.
- [21] D. Symons, private communication.
- [22] C. Kittel, *Introduction to Solid State Physics*, 6th edition, John Wiley & Sons, New York, 1986, pg. 167-171.

- [23] M. G. Burt, J. Phys. Cond. Matt. **4** (1992) 6651.
- [24] Landolt-Börnstein, *Numerical data and functional relationships in science and technology, New series group III, vol 17a*, edited by O. Madelung, Springer-Verlag, 1982, pages 258-278 and pages 297-310.
- [25] E. Merzbacher, *Quantum Mechanics*, 2nd edition, John Wiley & Sons, New York, 1970, page 356.
- [26] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures*, Halsted Press, John Wiley & Sons, New York, 1988.
- [27] P. Voisin, G. Bastard, M. Voos, Phys. Rev. **B 29** (1984) 935.
- [28] R. Q. Yang, J. M. Xu, and M. Sweeny, Phys. Rev. **B 50** (1994) 7474.
- [29] N. F. Johnson, H. Ehrenreich, P. M. Hui, and P. M. Young, Phys. Rev. **B 41** (1990) 3655.

Chapter 3

Cyclotron Resonance

In this chapter I describe cyclotron resonance (CR) experiments performed on InAs/(Ga,In)Sb superlattices. The basic CR experimental setup is described, then the theoretical elegance of the physics of CR is outlined. Three phenomena were investigated using CR: the nonparabolicity of the electron effective mass as a function of sample geometry and carrier density, the anisotropy of the hole effective masses in different growth directions (namely [001] and [111]), and oscillations in linewidth and intensity that can occur in heterojunctions.

3.1 INTRODUCTION	49
3.2 EXPERIMENTAL SETUP	49
3.3 THEORY	50
3.4 EXPERIMENTAL RESULTS	54
3.5 ANISOTROPIC VALENCE BAND MASSES	60
3.6 CONDUCTION BAND NONPARABOLICITY	65
3.7 OSCILLATIONS IN LINEWIDTH AND INTENSITY.....	68
3.8 CONCLUSIONS.....	73
3.9 REFERENCES	73

3.1 Introduction

Cyclotron resonance (CR) is one of the oldest and most widely-used experimental techniques of semiconductor physics. As discussed in Chapter 2, unexplained transitions in early bulk CR data were the motivation for the development of $k \cdot p$ theory [1]. CR was one of the first optical experiments to be performed on bulk materials [2] due to the straightforward set-up involved, and it continues to be used for two reasons: the analysis is very elegant, and CR is a powerful tool in the investigation of novel heterostructures as well as bulk materials. The experimental and theoretical aspects of cyclotron resonance will be detailed below.

Although much band information can be extracted from CR experiments, there is one quantity of paramount interest: the “effective mass” of the carriers involved in the transitions. Standard CR experiments exhibit transitions whose peaks shift linearly with applied magnetic field, and the effective mass of the transitions is therefore assigned as the inverse of the proportionality constant between the transition energy and magnetic field (the full theoretical justification for this is given below).

3.2 Experimental Setup

Summers [3] and Michels [4] give excellent descriptions of the experimental setup used for CR measurements, as well as details about the operation of the Bruker 113v Fourier transform infrared spectrometer. I will therefore only summarize, and highlight the important details for the purposes of my experiments.

Although the basics of the experiment have not changed in the forty-five years of CR history, the actual equipment used has changed quite a bit. The experiments presented here used 14 or 17 Tesla superconducting magnets. While early experiments were restricted to microwave frequencies, due to the weak magnetic fields available at the time, modern magnets allow us to work in the far and mid-infrared (20 to 500 cm^{-1} , or 3 to 60 meV). Irradiation of the sample, and the processing of data, is handled by a computerized Fourier transform infrared spectrometer. The transmission of the sample is measured by a silicon bolometer, mounted a few centimeters below the sample (out of field center). The sample and bolometer are held in an insert in a cryostat, with an operating temperature of 2K (I therefore call this the “2K insert”). Low temperatures were achieved by immersion in liquid helium, with a portion of the helium (the lambda-point refrigerator) being pumped to bring the liquid to its superfluid

λ -point. We found that a slight quantity of helium exchange gas in the insert (3-5 mbar at room temperature) gave optimum bolometer response, and fast cooling times.

Some measurements in this chapter were performed with a helium-3 insert, also described by Summers [3] and Michels [4]. Essentially, this insert contains the isotope ^3He , whose lower vapor pressure allows one to reach temperatures as low as 350 mK. For these experiments, however, we found the low temperatures unnecessary, and the extra work required for dealing with the ^3He (and the extra optical window limitations) were generally not worth the effort.

A polished brass light pipe was used to couple the infrared light from the spectrometer to the insert. An optical window must be placed at the junction of the light pipe and insert to maintain a vacuum in the insert. The light source used in the spectrometer, and the characteristics of the optical window, therefore determined what wavelengths of light reached the sample. For these experiments, the sources used were either a Mercury arc lamp (far-infrared, 0-700 cm^{-1}) or a simple blackbody globar (mid-infrared, 20-6000 cm^{-1}). The Hg lamp was used for close examination of hole resonances, otherwise we found the globar to give sufficient illumination at all wavelengths of interest. We used a polyethylene window throughout, which transmitted all light from 0-1000 cm^{-1} . For the ^3He insert, an additional sapphire window is placed before the bolometer, with a transmission range of 0-300 cm^{-1} . At the end of the light pipe, a parabolic focusing cone (Winston cone) focused the light onto the sample [3,4].

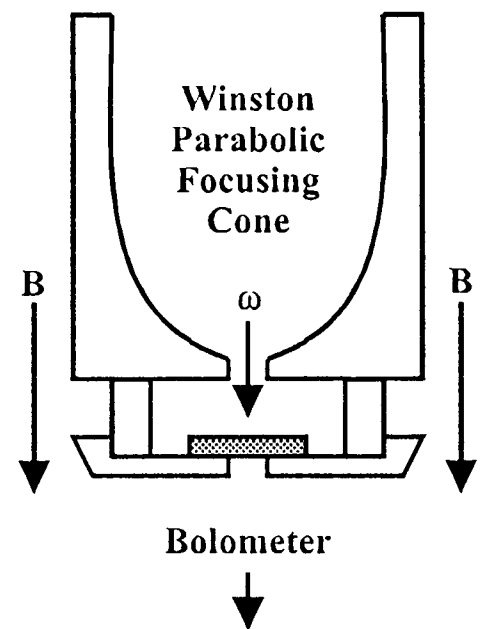


Figure 3.1: The end of the 2K insert, with the sample mounted in the Faraday configuration.

The sample itself is placed at field center, in the Faraday configuration (incident light and magnetic field are normal to the surface), as illustrated in Fig. 3.1.

3.3 Theory

In Chapter 2, where the case of applied magnetic field was first handled in a quantum-mechanical way, it was determined that only a field in the growth direction of a heterostructures could be described easily. The reason for the ease of mathematical description was that for a field in the growth direction, the quantizing effects of the heterostructure and field potentials were separable. This meant that the bulk magnetic field

Hamiltonian matrices could be calculated relatively easily for arbitrary growth directions, and as a result the electronic structure of heterostructures could be calculated including band coupling and field effects.

Unfortunately, a general multi-band discussion does not do justice to the real theoretical elegance of a field in the growth direction. This descriptive simplicity is worth discussing in a little more detail, as it plays an important role in the analysis of the experimental results.

In the effective mass approximation (EMA) as described in Chapter 2, the form of the Schrödinger wave equation (SWE) with arbitrary magnetic field becomes

$$\left[E_u^{(0)} + \frac{(p + eA)^2}{2m_u^*} + g_u \mu_B \mathbf{B} \cdot \boldsymbol{\sigma} \right] f(\mathbf{r}) = E f(\mathbf{r}), \quad (3.1)$$

where u denotes the Bloch function which is modulated by the envelope function, $E_u^{(0)}$ is the Γ -point energy of the u state, m_u^* is the carrier effective mass, and g_u is the spin-splitting g-factor for the u state, which will in general depend not only on u but also upon the confinement energy E . For the purposes of these experiments, g_u is largely ignored as spin-splitting is not experimentally resolved except for a few samples at high magnetic fields. The dependence of u on the carrier type is given in Table 3.1 below. To simplify the following discussion, I shall drop the subscript u , where it is understood that different carrier types will require different effective masses and Γ -point energies.

For a growth-direction field with vector potential $A = (yB, 0, 0)$ (this is the Landau gauge, chosen to be a simple form with $\nabla \cdot A = 0$), Eq. (3.1) becomes

$$\left[E^{(0)} + \frac{p^2}{2m^*} + \frac{e^2 B^2 y^2}{2m^*} + \frac{p_x e B y}{m^*} + V(z) \right] f(\mathbf{r}) = E f(\mathbf{r}). \quad (3.2)$$

Table 3.1: Effective mass parameters for various carrier types. E_C and E_V are the conduction and valence band energies at the Γ -point, respectively.

Carrier Type	Kane Basis State $ u\rangle = j, m_j\rangle$	Effective Mass m_u^*	Γ -point Energy $E_u^{(0)}$
electrons	$ 1/2, \pm 1/2\rangle$	m_e^*	E_C
heavy holes	$ 3/2, \pm 3/2\rangle$	m_{hh}^*	E_V
light holes	$ 3/2, \pm 1/2\rangle$	m_{lh}^*	E_V

By writing the general envelope function $f(\mathbf{r})$ as a combination of three functions

$$f(\mathbf{r}) = f(z) e^{ik_x x} \phi(y) , \quad (3.3)$$

Eq. (3.2) may be separated into two separate linear differential equations, one describing the growth direction quantization

$$H(z) f(z) = [E^{(0)} + \frac{p_z^2}{2m^*} + V(z)] f(z) = E_z f(z), \quad (3.4)$$

and one describing the in-plane confinement due to the field

$$H(y) \phi(y) = [\frac{p_y^2}{2m^*} + \frac{e^2 B^2 y^2}{2m^*}] \phi(y) = E_y \phi(y) . \quad (3.5)$$

In deriving Eq. (3.5), a canonical transformation of coordinates was made to eliminate the $y p_x$ cross term. The transformation amounts to a simple choice of the y -coordinate origin. Note that the Landau gauge $\mathbf{A} = (0, xB, 0)$ could also have been chosen, in which case the coordinates x and y would change places in the above equations, although the resulting energies would remain the same. This arbitrary choice of gauge merely reflects the isotropy of the problem in the x - y plane.

Eq. (3.4) is the Γ -point EMA SWE describing the quantization effects of the heterostructure. By solving Eq. (3.4), each subband i will then have its own envelope function $f_i(z)$ and bound state energy $E_{zi} = H(z) f_i(z)$.

Eq. (3.5) is the famous simple harmonic oscillator SWE, with equally-spaced eigenenergies

$$E_{yn} = (n + 1/2) \hbar \omega_c , \quad (3.6)$$

where the cyclotron frequency ω_c has the simple definition

$$\omega_c = \frac{e B}{m^*}. \quad (3.7)$$

The eigenfunctions (envelope functions) of Eq. (3.5) are the standard Hermite polynomials modulated with a rapidly decaying exponential, written explicitly (with normalization constants) as

$$\phi_n(y) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m^* \omega_c}{\hbar \pi} \right)^{1/4} \exp\left(-\frac{m^* \omega_c}{2 \hbar} y^2 \right) H_n\left(\sqrt{\frac{m^* \omega_c}{\hbar}} y \right), \quad (3.8)$$

where H_n is the Hermite polynomial of order n .

From Eqs. (3.6) and (3.4), one finds that the energy of a carrier in subband i , Landau level n , is then

$$E_{in} = E_{zi} + E_{yn} = E_{zi} + (n + 1/2) \hbar \omega_c, \quad (3.9)$$

a simple linear combination of the energies in the different directions. In the EMA, the simplifying effect of a growth-direction field is obvious: the SWE of Eq. (3.1) completely decouples, the energies and momenta of the growth and layer plane directions being independent.

The simplicity of the growth-direction field is even more evident when one considers transitions. From the selection rules derived in Chapter 2 (Eq. (2.50)), it is seen that for normally incident light (light polarized in the plane of the layers) in the EMA, only absorption between adjacent Landau levels of the same subband is allowed. For the simple form of the SWE in Eq. (3.1), this means that there will be only one absorbed frequency per carrier type, namely ω_c , the cyclotron frequency defined in Eq. (3.7).

Therefore, for any observed cyclotron resonance of energy ω_c , an effective mass is defined using Eq. (3.7). The theoretical justification for such a definition in the InAs/GaSb system is weak, as the strong interband mixing is expected to inhibit the decoupling of the SWE. Nonetheless, it is seen experimentally to be a useful characterization of magnetic field transitions, which display a striking linear dependence on field. Even for the valence band, where the strongest band-mixing is expected, resonances are approximately linear in field. For

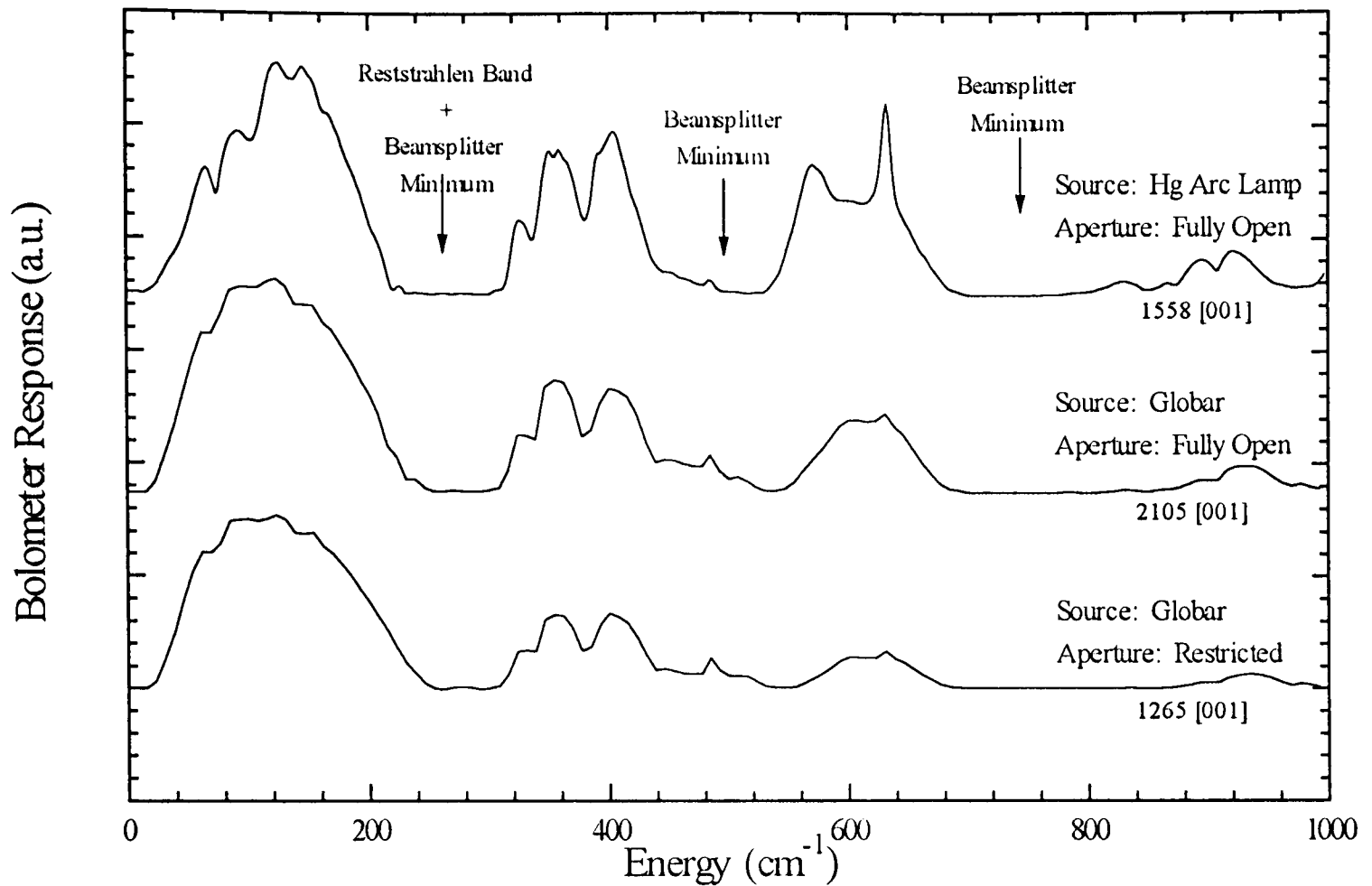


Figure 3.2: Raw bolometer response at 14 Tesla for three different samples. All traces are from the same insert, using the same beamsplitter and optical windows. Only the source and aperture are changed.

the rest of this chapter, I will talk about effective masses corresponding to observed absorption peaks in CR experiments.

3.4 Experimental Results

As mentioned in the experimental setup described above, the detector used was a silicon bolometer, mounted behind the sample in the insert, positioned some distance out of field center. Our early experiments used an insert with a bolometer sitting close to the field center, which lead to field-dependent bolometer response. Later experiments used a modified insert with a slightly longer tail, moving the bolometer several centimeters out of the field, and little field-dependence remained.

Using a Fourier spectrometer, the standard CR technique is to hold the magnetic field at some fixed value, and then take an average of several hundred spectra to arrive at the “final” field spectrum. The end result for each sample is then a series of bolometer response spectra, one for each field value. The bolometer response will be complex, depending on the spectral output of the spectrometer light source, the transmission of the optics and light pipes, the characteristics of the various optical windows, the thickness, quality and composition of

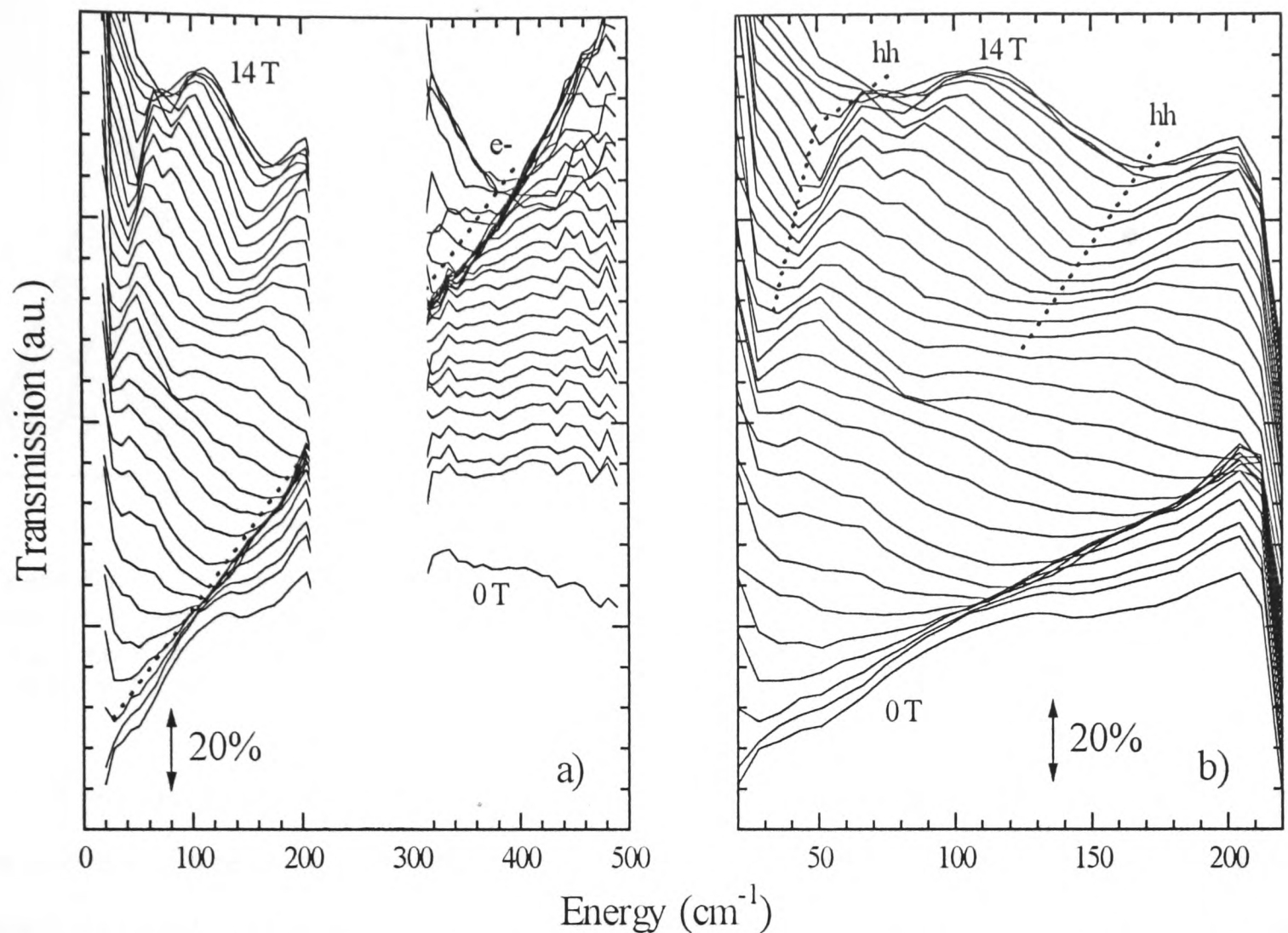


Figure 3.3: Spectra for sample 1546 [001], ratioed against a GaSb buffer layer (1996 [001]). The traces start at the top at 14 T, and decrement in $\frac{1}{2}$ T steps. The blank area from 220-300 cm^{-1} is the reststrahlen band of GaAs (the substrate). Plot b) is simply a close-up of the low-energy region, showing the hole resonances more clearly. The lines are a guide to the eye.

the sample, and might possibly also contain the desired electronic resonances. The question is how best to remove the background of the spectra, and focus only on resonances.

The most common method of removing the background is to ratio the spectra against the zero-field response of the sample. The only difference between the two traces is the field value, hence the only deviation from unity in the ratio should be field-dependent effects, hopefully CR transitions. This is a particularly useful technique when looking at high-field transitions, or samples with low carrier densities.

However, the technique can fail for resonances occurring at low energies (large effective masses, such as hole transitions) or for samples with high carrier densities. The problem is that the large free carrier absorption at zero field “skews” the spectra, resulting in a sharp rise near zero energy. Low-energy transitions appear as small dips on the slope, often shifted from their “true” position, and can be difficult to distinguish from noise. An alternative is to ratio the spectra against some other field value (e.g., ratio the 14 T trace against a 5 T trace), but the pitfall here is that resonances in the reference spectra may shift features in the signal.

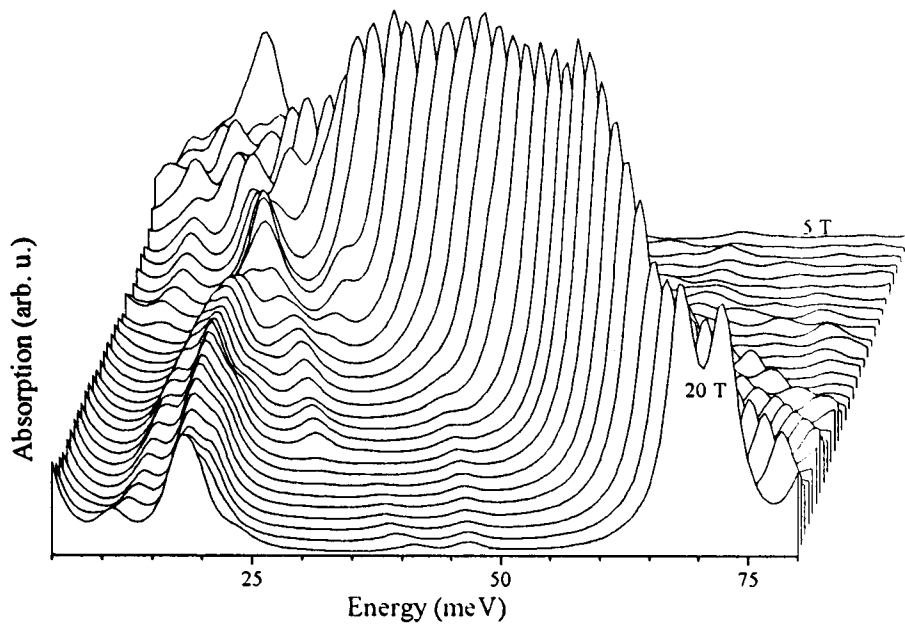


Figure 3.4: Calculated CR for a 200 Å InAs/80 Å GaSb superlattice, with self-consistency included (carrier density $n = p = 4 \times 10^{11} \text{ cm}^{-2}$). The traces start at the top at 5 T, and increase in 1 T steps.

A third ratioing technique is to perform the identical experiment on a sample with no carriers at all (a GaSb buffer layer, in our case). Here there are no problems with resonances in the reference spectra, but care must be taken to ensure that all experimental conditions are the same for both the sample and reference measurements. There are a number of parameters when using a Fourier spectrometer, including source used, mirror velocity, aperture

and filters used, and beamsplitters, to name the most common. Also, even for identical parameters, the response can change over time, as light pipes may be cleaned or become dirty, windows may be replaced, *etc.* We find in practice that the reference spectra should be taken within a few days or weeks within taking the sample spectra. When done carefully, referencing against a buffer layer provides clear resonances at almost all field values.

In practice, all three techniques were used in analyzing the data presented here. Different samples required different ratioing methods, but care was taken to ensure that different methods resulted in comparable resonance positions and intensities.

Typical experimental traces are presented in Fig. 3.3. Due to the presence of large electron and hole populations, several resonances can be seen in most structures. All semi-metallic samples (superlattices and double-heterojunctions) exhibit electron resonances, with a corresponding effective mass of $(0.03 \pm 0.01) m_0$. In superlattices, hole resonances are also observed. Two hole resonances are usually observed: one with a mass of $(0.25 \pm 0.05) m_0$ (heavy holes), and one with a mass of $(0.08 \pm 0.02) m_0$. The intensities of the two hole resonances appear to be a complex function of sample geometry and field strength, but in general both resonances are observed in any sample with a large population of holes (*i.e.*, any superlattice). It is tempting to ascribe the lighter hole mass to light holes, but all single-band and multi-band calculations agree that light hole levels will not be populated in any of these structures. Transport measurements confirm that the only populated hole states are heavy holes. Lakrimi *et al.* [5] have shown that the resonances are not due to magnetoplasmon effects.

Therefore the two hole resonances are attributed to heavy holes. First observed in the GaAs/AlGaAs system [6], the dual heavy hole resonance has been reproduced in valence band $k \cdot p$ calculations [7,8]. Essentially, the resonances arise from the different masses of the spin states. The spin up state results in a transition mass close to the heavy bulk value, while the spin down state tends to give a lighter effective mass, approximately half the mass of the spin up state. In GaAs/AlGaAs heterojunctions [6], the splitting is due simply to a lifting of the Kramers (spin) degeneracy due to the inversion asymmetry of the structure, and not to any effect of the magnetic

field. Inversion asymmetry has been evoked to explain splitting in electron resonances in InAs/(Al,Ga)Sb quantum wells [9,10]. Luo *et al.* [9] demonstrate that asymmetry splitting is most likely due to electric field effects, and not to the underlying bulk asymmetry of III-V materials. Both Luo and Warburton [10] observe their asymmetry-induced splitting in single InAs quantum well structures, where surface effects are expected to provide a non-zero electric field in the growth direction [11]. Fig. 3.4 shows a calculation of the CR of a semimetallic InAs/GaSb superlattice (see Chapter 7). Two heavy hole resonances are observed, with masses of 0.21 and 0.12 m_0 . The electron resonance has a mass of around 0.034 m_0 , with spin-splitting becoming resolved at high fields (a constant broadening of 3.5 meV has been assumed in the model). In this case, at 20 T only one heavy hole Landau level is populated, and the two hole resonances are due to absorption at $k_z = 0$ and π/d , although in general the heavy hole resonances observed in other samples can also be attributed to different spin states, depending on population effects.

Given that as many as three resonances may be observed in a single sample, the next step in the analysis is to plot the resonance frequency positions versus their magnetic field values. The result is a “Landau fan,” as in Fig. 3.5. Given the basic CR equation of Eq. (3.7), one would expect the resonances to all extrapolate back to zero energy at zero field. This is

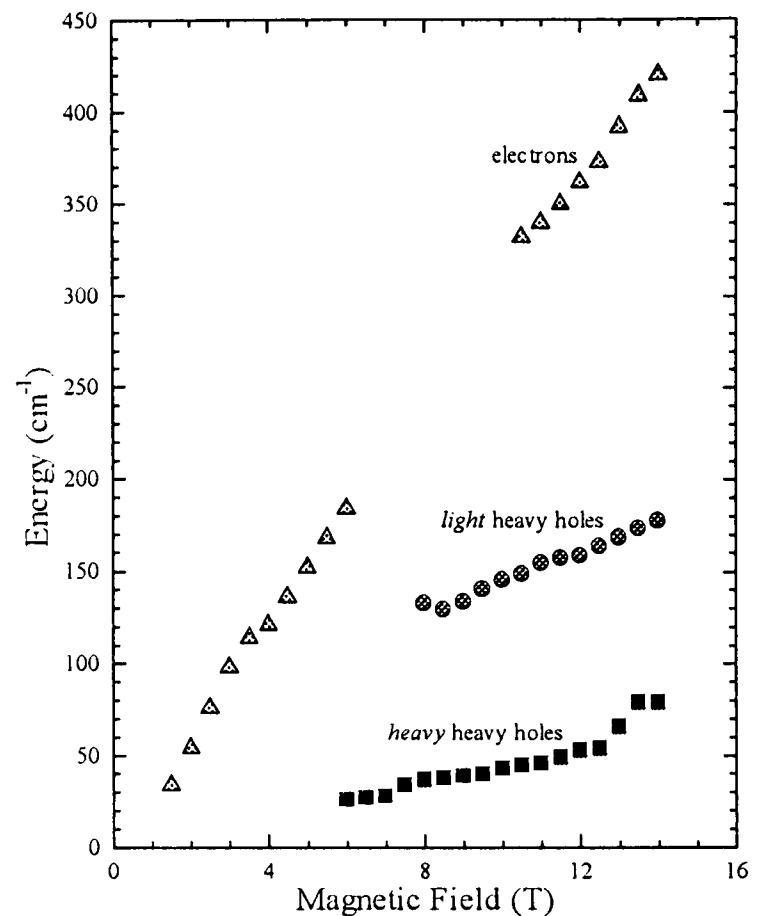


Figure 3.5: The Landau fan (resonance energy vs. field position) for sample 1546 [001], displaying electron and hole resonances.

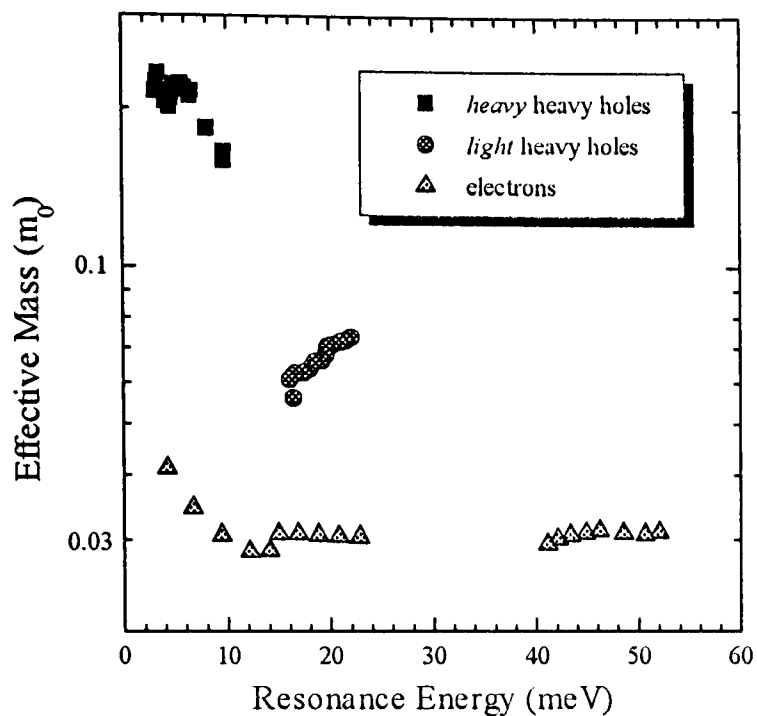


Figure 3.6: Effective masses for sample 1546 [001].

dispersion of the effective masses. In the case where the Fermi level is roughly constant with respect to magnetic field (expected to hold for the samples under study here), the effective masses are expected to remain constant as well, and this is usually observed, although again the hole masses tend to be somewhat field-dependent, due to the complexity of the valence band Landau level structure.

The observed electron masses are very much enhanced over the band-edge value of $0.023 m_0$ [12], as predicted by nonparabolicity. Sakaki *et al.* [13] performed the very first CR experiments in InAs/GaSb superlattices, finding masses varying between 0.048 and $0.068 m_0$, for both semimetallic and semiconducting samples. Subsequent experiments by Bluysen *et al.* [14] on a semiconducting sample found effective masses of around $0.043 m_0$, and it is these slightly higher masses which tend to be observed in modern samples.

Guldner *et al.* [15] and Maan *et al.* [16] found electron effective masses of around $0.038 m_0$, with wide layer (semimetallic) superlattices. These were the first CR experiments to see hole resonances, giving a mass of $0.26 m_0$. This mass is lighter than the generally accepted GaSb bulk mass of $0.33 m_0$, but agrees with other GaSb measurements [17]. The Guldner-Maan data also exhibited apparent interband resonances, that is, $\Delta n = 0$ transitions between heavy hole and electron states. These transitions indicated negative band gaps on the order of -50 meV, in agreement with theory. Analysis of the interband data provided a measurement of the miniband width (~ 20 meV) of the lowest conduction band state, again in good agreement with theory.

observed to be the case in all electron resonances. Hole resonances sometimes did not extrapolate back to zero, but low field resonances were difficult to obtain, and we expect the extreme anisotropy of the valence band to result in field-dependent masses [7,8].

With the Landau fan thus established, Eq. (3.7) is applied to extract an effective mass for each observed transition. The masses are then plotted as a function of their resonance energies (Fig. 3.6), describing the resonance

A number of studies have been performed on electron CR in thin InAs layers sandwiched between $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ barriers [18-21]. These studies focused on oscillations in the resonance linewidth, intensity, and effective mass, and more will be said of them later in the chapter. Electron effective masses were in the range of 0.032 to 0.042 m_0 , consistent with the above results, and no hole resonances were observed. Kim *et al.* [22] found very large electron (0.037 to 0.056 m_0) and hole (0.36 m_0) masses in InAs quantum wells with GaSb barriers, including both semiconducting and semimetallic structures.

CR studies of InAs/GaSb superlattices grown here at the Clarendon [5,23] have shown consistently lighter electron effective masses (0.032 m_0 on average) than most studies above, although our [001] hole mass of around 0.26 m_0 is in good agreement with previous findings. Most of the electron effective mass discrepancy can be explained by differences in carrier density. All *non*-Clarendon studies have used MBE-grown samples, and all show significant

Table 3.2: Samples measured in these experiments. Under “Period,” the InAs layer thickness is listed first. N is the number of periods in the superlattice. Carrier densities are taken from 4.2 K transport measurements, in units of 10^{11} cm^{-2} . The lowest-lying electron level (E_0), highest hole state (HH_0), and Fermi level (E_F) are from a self-consistent single band calculation, where the conduction band minimum is taken as the zero of energy.

Sample	Period Å	N	In %	n	p	m_e^* m_0	m_{hh1}^* m_0	m_{hh2}^* m_0	E_0 meV	HH_0 meV	E_F meV
1132 [001]	190/190	20	0	7.0	3.1	0.035	0.28	0.06	57	132	129
[111]	145/295			10.4	2.6	0.038	0.19	0.085	106	220	218
1133 [001]	190/85	20	0	2.97	0	0.035	0.25	0.075	57	128	127
[111]	145/170			10.7	3.6	0.039	0.16	--	104	214	212
1249 [001]	220/120	20	0	6.5	6.2	0.032	0.24	0.08	51	125	120
[111]	180/120			10.9	5.4	0.039	0.16	0.07	92	209	205
1252 [001]	100/50	20	0	--	--	0.038	--	--	112	106	109
[111]	75/75			--	--	0.042	--	--	188	180	184
1263 [001]	450/100	20	16	12	11	0.032	0.27	0.09	75	148	138
[111]	310/202			18	9	0.035	0.19	0.075	136	270	263
1265 [001]	450/100	20	10	8.7	7.6	0.029	0.27	0.065	70	138	129
[111]	310/202			16.5	8.5	0.031	0.19	0.08	126	241	236
1266 [001]	450/100	20	10	11	10	0.031	0.26	0.045	70	138	129
[111]	310/202			16	10.1	0.033	0.19	0.06	123	235	229
1269 [001]	405/85	20	10	8.2	5.2	0.033	0.20	0.10	69	140	134
[111]	395/110			16.2	9.2	0.035	0.18	0.08	123	224	218
1296 [001]	260/75	20	4	7.5	3.4	0.031	0.27	0.06	55	133	130
[111]	170/130			15.1	6.2	0.033	0.20	0.08	106	219	216
1546 [001]	465/108	20	0	7.2	4.6	0.031	0.21	0.07	65	124	119
1558 [001]	465/108	20	0	8.1	4.8	0.028	0.17	0.072	66	125	120
1590 [001]	155/90	100	0	4.2	--	0.036	0.17	0.075	68	130	129
2028 [001]	220/180	20	0	7.0	6.9				51	124	118
2064 [001]	220/180	20	0	7.3	7.2	0.035	0.20	0.075	51	124	118
1179 [001]	300/∞	DHET	0	7.5	--	0.036	--	--			
2056 [001]	1000/∞	DHET	0	10.8	--	0.030	0.34	--	71	132	130
2105 [001]	400/∞	DHET	0	7.6	--	0.030	--	--	66	132	130
2117 [001]	?/∞	DHET	0	9.4	--	0.031	--	--	69	133	131

n-type behaviour. The extremely heavy masses of $\sim 0.06 m_0$ found by Sakaki *et al.* [13] and Kim *et al.* [22] were for samples with thin InAs thicknesses, and carrier densities approaching 10^{12} cm^{-2} . The Fermi level for such systems is therefore several hundred meV above the band edge, and so it is no surprise that heavier masses are found.

In contrast, the Clarendon samples are grown by MOVPE (discussed in Chapter 1), with near-intrinsic carrier densities. Thin layer samples (discussed in Chapter 6) froze out at low temperatures, with effective masses determined from interband measurements to be $\sim 0.04 m_0$. When the intrinsic nature of the Clarendon samples is taken into account (*i.e.*, comparing carrier densities as well as layer thicknesses), we find our electron effective masses to match previous studies. Only in our intrinsic samples, with large hole populations, are two heavy hole resonances observed.

The samples used in these studies, as well as extracted effective masses, are listed in Table 3.2. Carrier densities were taken from magneto-transport experiments performed at 4.2 K. A self-consistent calculation in the effective mass approximation (see Chapter 2) was carried out for these samples, with the resulting energy levels displayed in Table 3.2 as well. Carrier densities predicted by the model were found to match transport values to better than 5% [5]. For this self-consistent model, the piezoelectric field was included for samples grown in the [111] orientation (for a review see ref. [11]).

3.5 Anisotropic Valence Band Masses

An examination of the bulk $k \cdot p$ matrices in the Appendix gives some idea how the effective masses of the carriers are likely to change with growth direction. The electron effective mass is expected to be isotropic, as the diagonal and electron-hole coupling terms do not change with orientation (a consequence of the spherical symmetry of the electron $|s\rangle$ state). The hole states, however, are expected to show some degree of anisotropy, as the diagonal and coupling terms change with orientation. This variation of hole mass with orientation has device consequences, as heavier hole states will be more susceptible to quantum confinement, and may allow growth of thinner GaSb barriers for a given band gap, which may improve absorption or emission properties. Clearly, it is useful to know how the masses change with growth orientation.

To arrive at an estimate of the carrier effective masses, the bulk Hamiltonians are examined in two limits (assuming for convenience that the growth direction momentum, k_z , is zero). In the first limit, the heavy holes and light holes are assumed to have decoupled (*e.g.*,

Table 3.3: In-plane heavy-hole masses for the [001] and [111] orientations. For the [001] orientation, the bulk mass is anisotropic within the plane. It is assumed that $k_z = 0$. Parameters used are $\gamma_1 = 14.3$, $\gamma_2 = 5.3$, and $\gamma_3 = 6.5$ (ref [26]). In the decoupled limit, the mass is slightly heavier in the [001] direction, while in the bulk limit, the mass is expected to be anisotropic, but the exact mass depends on the dispersion in the plane.

Orientation	Bulk Limit (lh-hh coupling)	Decoupled limit
[001]	$k_{ } = (k_x, 0) \text{ or } (0, k_y) : (\gamma_1 - 2\gamma_2)^{-1} = 0.27 m_0$ $k_{ } = (k, k) : (\gamma_1 - 2\sqrt{\gamma_3^2 + \gamma_2^2})^{-1} = \infty$	$(\gamma_1 + \gamma_2)^{-1} = 0.051 m_0$
[111]	$(\gamma_1 - \sqrt{3\gamma_3^2 + \gamma_2^2})^{-1} = 0.54 m_0$	$(\gamma_1 + \gamma_3)^{-1} = 0.048 m_0$

due to strain or confinement effects). In this case, one can extract the dispersion from the diagonal of the matrix. In the second limit, bulk dispersion is calculated, which requires the diagonalization of a 2x2 matrix for the [001] case, or a 4x4 matrix for the [111] case. The heavy-hole eigenvalues of the reduced matrix then give the effective mass. The results are given in Table 3.3 above. The most important result is that different effective masses for the [001] and [111] orientations are expected.

The exact masses given in the table are of dubious validity. Particularly in a heterostructure, k_z is definitely nonzero due to confinement effects. One certainly never sees experimentally the light masses predicted by the decoupled limit, as extreme separation between heavy holes and light holes is difficult to achieve. And coupling between the conduction and spin-orbit bands has been neglected, which are near to the valence band in InAs/GaSb structures (although the values of the γ 's used are the actual (not modified) Luttinger parameters, hence implicitly include conduction band coupling). The infinite mass given in the [110] dispersion for the [001] orientation is an artifact resulting from the particular choice of γ values, and in general the mass in the [110] direction is not drastically enhanced over the [010] or [100] directions, as is evident from Fig. 2.3. Nonetheless, the basic result of growth-direction anisotropy remains.

Warburton *et al.* [25] observed anisotropic hole masses in the $\text{In}_x\text{Ga}_{1-x}\text{Sb}/\text{GaSb}$ system. They found the [111] hole mass to be lighter than the [001] mass by around 20%. Their heavy hole masses were closer to the decoupled limit than the bulk limit, which was attributed to the high strain of their system. In addition, they observed two heavy hole resonances for samples with high hole densities.

To observe this anisotropy the InAs/(In,Ga)Sb system, a number of superlattices were measured. The superlattices were grown with [001], [111]A and [111]B substrates placed side-by-side in the growth reactor, so that ideally the growth conditions and layer thicknesses would be identical for the two orientations. In practice, the [111] growth rates were different

from [001]: the [111] InAs layers were 30% thinner, and the GaSb layers almost twice as thick as the [001] layers. However, given that the lowest-lying hole states (the only states populated) are relatively insensitive to the exact layer width, the discrepancy in layer thicknesses is not expected to obscure the results.

The [111]A and [111]B notations refer to the two crystallographic directions: [111]A = [111] and [111]B = $[\bar{1}\bar{1}\bar{1}]$. In the z-direction of [111] samples, there is a large gap (of width $\sqrt{3}a/4$ where a is the lattice constant) between closely spaced planes (spacing $\sqrt{3}a/12$) of III-V elements. For [111]A samples, the growth order is ...V-III-gap-V-III-gap..., whereas in [111]B samples the order is ...III-V-gap-III-V-gap.... Transport measurements indicate that the [111]A and [111]B samples have similar carrier densities, but the [111]A samples gave consistently better electron mobility. Therefore, in the rest of the discussion, when I refer to measurements on [111] samples, I am referring to [111]A samples (see ref. [11]).

The concentration of indium varied from sample to sample, which had the effect of varying the barrier band gap and lattice constant, as well as the band overlap. Therefore, the samples had a wide range of strain and piezoelectric fields. Likewise, because of the variation of layer widths and band overlaps, a wide range of carrier densities and n/p ratios was observed in transport.

Twenty superlattices were measured, ten samples with one measurement for each substrate orientation. The results were conclusive: the electron mass, as expected, was isotropic, and the [111] *heavy* hole mass was 25% lighter than the [001] hole mass, for all samples studied. The *light* heavy hole mass also varied with orientation, but not in any obviously systematic way. This anisotropy of 25% is close to that observed by Warburton *et al.* [25], which is not surprising considering the similarity of the material systems. Our observed heavy hole masses are midway between the bulk and decoupled limits,

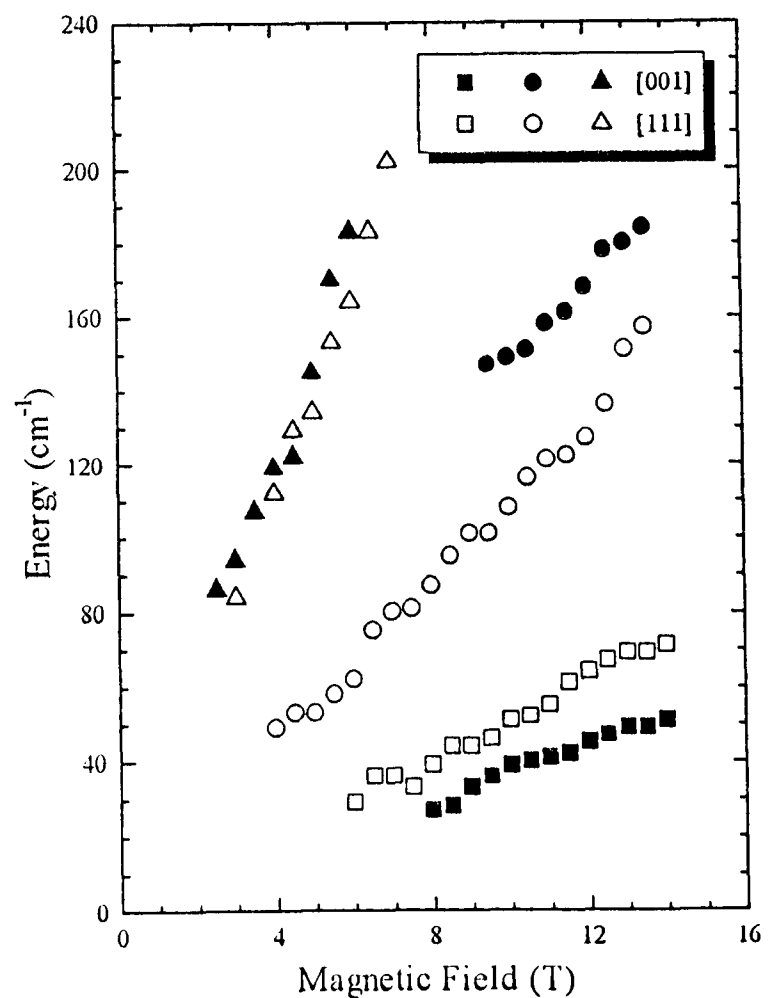


Figure 3.7: The Landau fan for sample 1266, for both the [001] and [111] orientations.

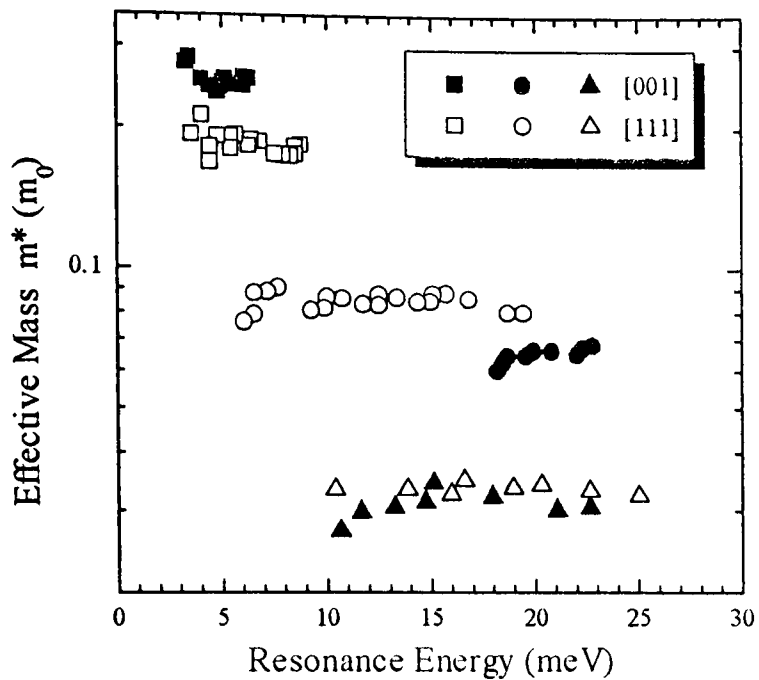


Figure 3.8: Effective mass vs. resonance energy for sample 1266, for both the [001] and [111] orientations.

as expected. The Warburton masses were much lighter, but again that is accounted for by the higher strain in their system.

Fig. 3.7 is a typical Landau fan, for sample 1266. Sample 1266 had large well widths and thinner barriers (the InAs/GaSb thickness ratio was 450Å/100Å and 300Å/200Å for the [001] and [111] orientations, respectively). One electron and two hole resonances are observed.

Fig. 3.8 is the effective mass dispersion for sample 1266. The [001] heavy heavy hole resonances have an effective mass of approximately $0.26 m_0$, while the [111] mass is around $0.19 m_0$. The electrons are basically isotropic, as expected, and for this sample the light heavy hole effective mass was around 20% heavier for the [111] orientation than [001].

Fig. 3.9 is the effective mass dispersion for sample 1132. Sample 1132 has different growth characteristics than 1266, with thinner InAs layers (and correspondingly less carriers), and thicker GaSb barriers (190Å/190Å for [001], 145Å/295Å for [111]). Nonetheless, the results are similar: the [111] heavy heavy hole masses are around $0.20 m_0$ compared to $0.27 m_0$ for [001], and the electron mass is essentially isotropic. In this case as well, the light heavy hole mass was heavier in the [111] orientation than [001], but again, this varied from sample to sample.

Since the heavy heavy hole effective mass shifts by almost the same amount for a wide range of indium concentrations (from 0 to 16%, see Fig. 3.10), the observed anisotropy is probably not due to the effects of strain or the piezoelectric field. In addition, the electron and hole densities vary widely from sample to sample, as does the electron to hole density ratio. The anisotropy is therefore probably not a consequence of the Coulombic band-bending

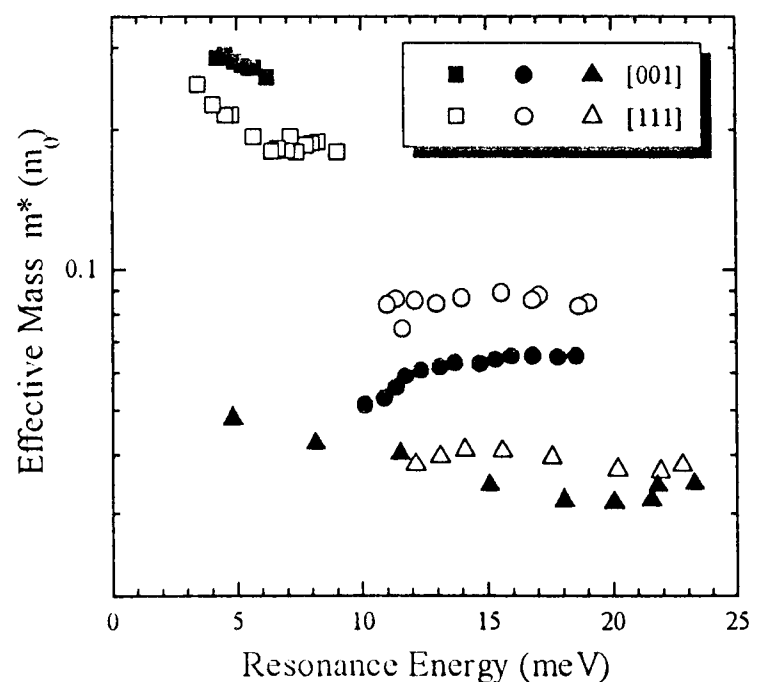


Figure 3.9: Effective mass vs. resonance energy for sample 1132, for both the [001] and [111] orientations.

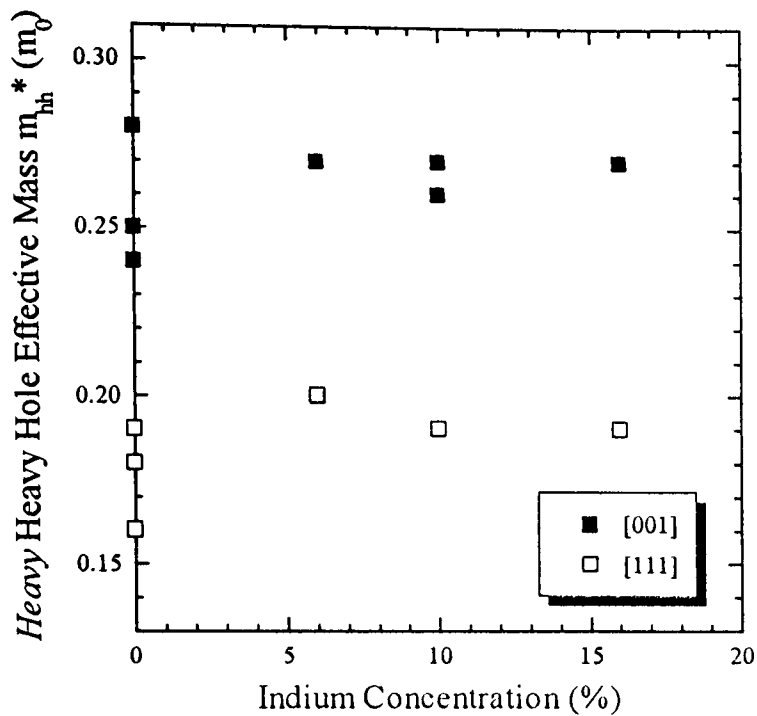


Figure 3.10: Heavy heavy hole masses for fourteen samples, plotted against the indium concentration of the barrier (some points lie on top of each other).

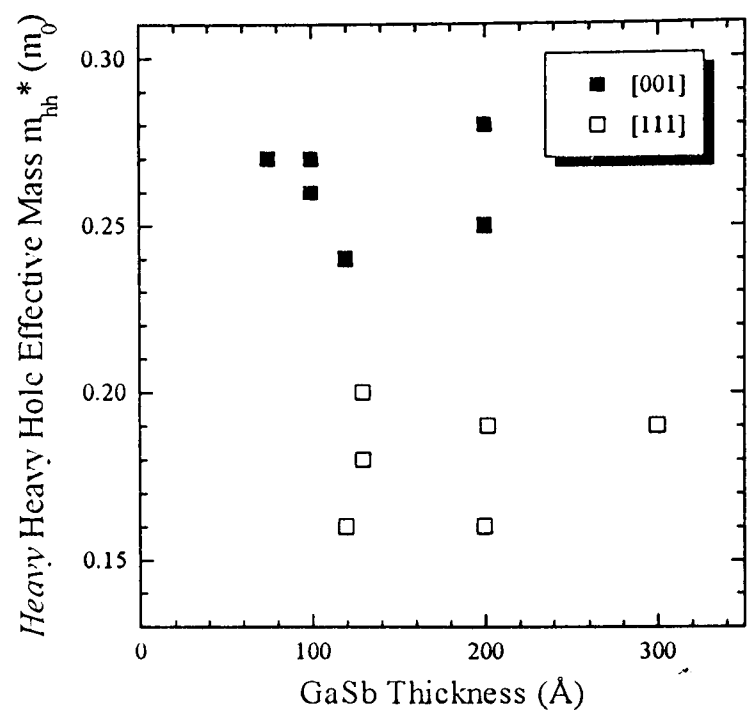


Figure 3.11: Heavy heavy hole masses for fourteen samples, plotted against the (In,Ga)Sb layer thickness (some points lie on top of each other).

either. The effective masses seem to be much more sensitive to growth direction than GaSb layer thickness (Fig. 3.11), so the anisotropy is not due to variations in layer thicknesses.

The superlattice *heavy heavy* hole effective mass anisotropy is attributed to the anisotropy of the bulk GaSb dispersion, that is, to the anisotropy of the bulk heavy hole $|^{3/2}, \pm^{3/2}\rangle$ basis state, and not to any sort of heterostructure confinement or strain effect. The observed masses are quite different from those listed in Table 3.3 (and indeed simple analysis of the Hamiltonian does not even predict which crystal orientation should result in lighter masses), therefore it is clear that these structures are far from either of the decoupled or bulk limits used in the table. Instead, InAs/GaSb superlattices place the heavy hole levels in the midst of electron and light hole levels, which results in complicated mixing between states (see the calculated Landau levels of Chapters 2 and 7).

The “spaghetti-like” Landau bands predicted by $k \cdot p$ theory can result in large, unobserved changes in effective mass with magnetic field. In practice it is suspected that different layers in the superlattice have slightly different band structures, due to local fluctuations in layer thickness, indium concentration, and interface quality. This results in a “smearing-out” of the resonance, where the observed transitions are a sum of the different individual transitions from each layer. The resulting effective mass will therefore be representative of the underlying heavy hole dispersion, rather than a consequence of particular band interactions at the Fermi level. This “smearing-out” effect certainly occurs for electron resonances, where in heterojunctions oscillations are observed in linewidth and intensity due to

bands crossing the Fermi level (discussed below), oscillations which disappear when superlattices are examined.

3.6 Conduction Band Nonparabolicity

As was mentioned in the EMA discussion of Chapter 2, all influences of farther bands are contained in the effective mass m^* of the carrier. Although the EMA is strictly valid only for constant m^* (the mathematical decoupling of motion in the growth and planar directions is impossible if $m^* \propto E$), in fact m^* shows a definite energy-dependence for almost all material systems. However, the EMA is still a good approximation, even for systems with fairly large nonparabolicity [27].

As the far bands become more distant in energy, their influence should decrease, leading to an increase in the effective mass (assuming that most of the influence is from the valence band, which is true of the InAs/GaSb system). Therefore, as conduction states move above the band edge, the mass should increase. For a heterostructure, this implies that bound states located further up the well should have heavier masses. An examination of the conduction band curvatures in Figs. 2.5 and 2.6 shows that this prediction of $k \cdot p$ theory certainly holds for semiconducting samples, and the tangled bands of Fig. 7.17 show the same behavior for a semimetallic sample under a magnetic field (the Landau levels of the E_i level are more closely spaced than those of E_0).

A number of samples have been measured over the past three years, mostly as part of other studies, such as the valence band anisotropy mentioned above or the coupled experiments covered in Chapter 5. However,

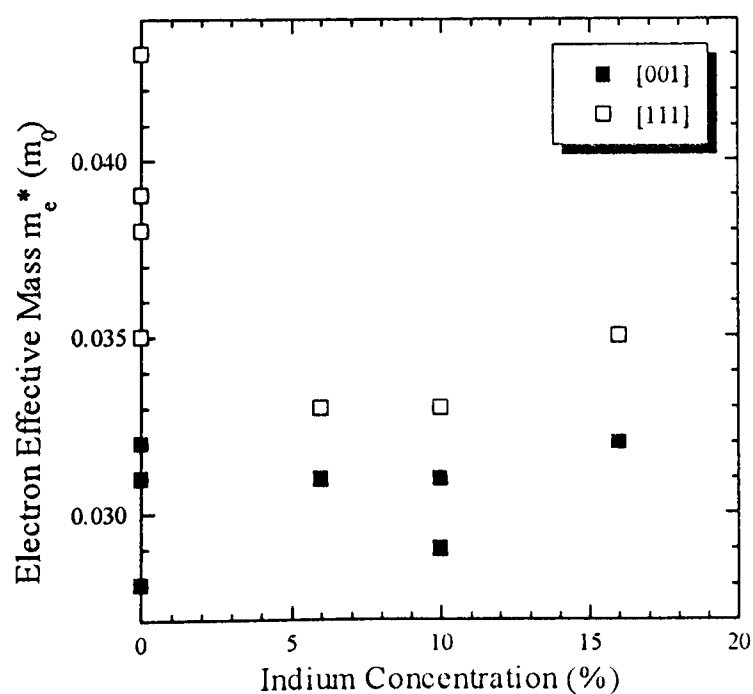


Figure 3.12: Electron effective mass as a function of indium concentration.

this large set of measurements allows for analysis of the electron effective mass, with a number of different sample variables such as layer thicknesses, carrier density, growth direction, and strain. The electron effective mass is observed to vary from 0.028 to 0.042 m_0 , variation which is attributed to the confinement effects of the InAs well.

The first plot, Fig. 3.12, shows the dependence of the effective mass with indium

concentration in the barrier. It is tempting to claim some sort of functional dependence on indium content, with the additional result that the mass is somewhat orientation-dependent, as the [111] masses appear about $0.002 m_0$ heavier.

The orientation dependence is unlikely for two reasons: first, the experimental uncertainty in the effective masses is not much less than $0.002 m_0$, the observed anisotropy, and second, the real difference is most likely due to differences in the layer thicknesses for

the two orientations. As was mentioned above, the [111]-grown samples had well widths reduced by some 30% below the [001] thicknesses, which would “squeeze” the conduction states to slightly higher energies, with correspondingly heavier masses. In addition, the [111] samples experience a larger band overlap [11], leading to a larger carrier density and so a larger mass at the Fermi level.

The slight indium concentration dependence is probably also due to confinement effects. The samples with Indium in the barrier were all grown with wide InAs wells (of width 400 Å or more). These wide wells have very low-lying electron levels, hence we expect the light effective masses which are constant for the range of nonzero indium concentration.

The possibility of orientation or indium concentration dependence is further refuted by examination of the mass as a function of InAs well width (Fig. 3.13). Unlike the valence band case of Fig. 3.11, here a strong dependence of effective mass on well width is observed. Likewise, the orientation dependence is negligible. As expected, a thinner InAs layer leads to a heavier effective mass, as a result of the higher confinement energy.

A further possibility is carrier concentration dependence. It is expected that for a fixed well width, increasing the carrier concentration will promote further Coulombic band-bending, forcing the bound states to higher energies and so resulting in heavier effective masses. Experimentally, however, the picture is somewhat clouded (Fig. 3.14). The problem is that for the undoped InAs/GaSb system, the only way to increase the carrier density is to grow thicker layers. This results in smaller confinement energies, allowing more charge transfer from the hole to conduction band. This increases the Coulombic band-bending, but at the cost

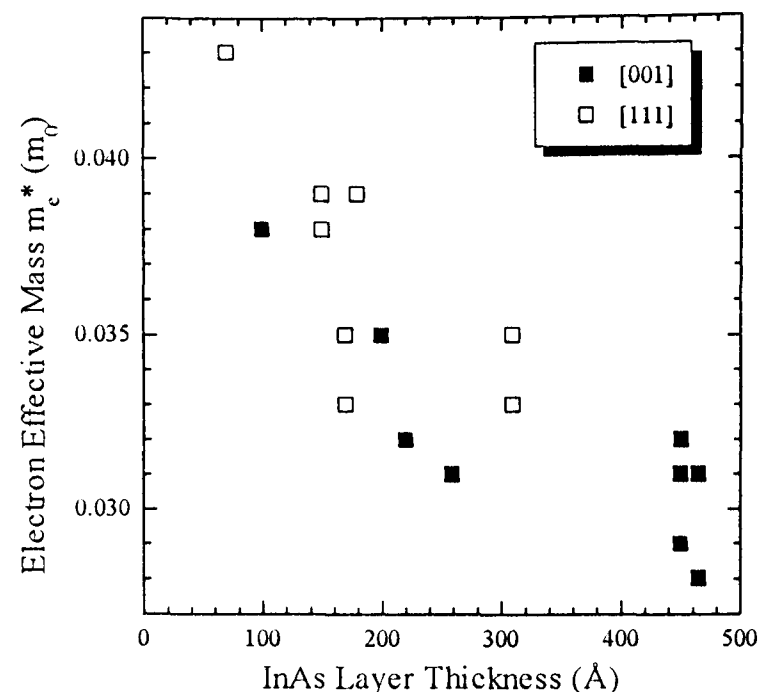


Figure 3.13: Electron effective mass as a function of InAs well thickness.

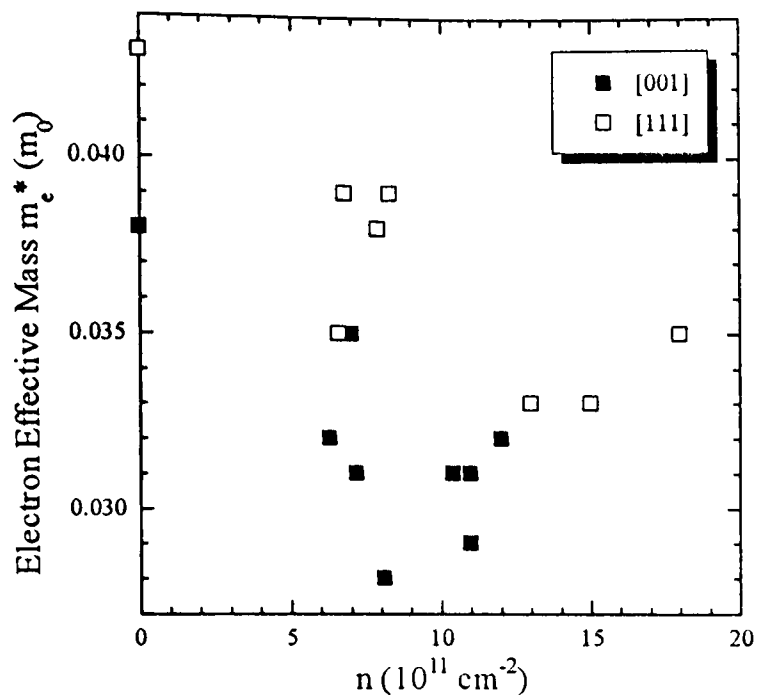


Figure 3.14: Electron effective mass as a function of carrier density.

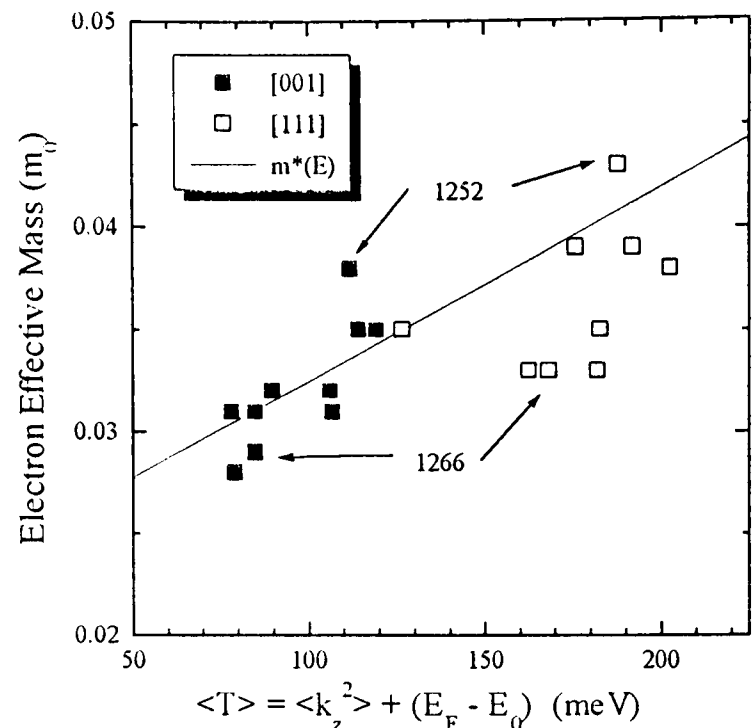


Figure 3.15: Electron effective mass as a function of the calculated kinetic energy at the Fermi level. The straight line is from a simple 3-band Kane model (Eq. (3.10)).

of widening the InAs well, allowing the bound states to settle into lower energies. A further complication is that [111] structures experience a larger band overlap, which for a given well width introduces more carriers. Comparing Figs. 3.13 and 3.14, one is led to the conclusion that carrier density (and so Coulombic band-bending) does not influence the bound states of the system (or the masses) as much as the InAs thickness.

To better understand the effects of quantum confinement on the effective mass, the electronic structure is calculated for the superlattices of Table 3.2. The plot of effective mass against Fermi level is given in Fig. 3.15. The straight line is from a simple 3-band Kane model [28] which has proven to be accurate in describing the InAs conduction band [11]:

$$m^*(E) = m_0^* \left(1 - 2 \kappa \frac{\langle T \rangle}{E_G} \right), \quad (3.10)$$

where $m^*(E)$ is the energy-dependent effective mass, m_0^* is the band-edge effective mass (0.023 m_0 for InAs), $\langle T \rangle$ is the kinetic energy measured above the band edge, κ is a nonparabolicity parameter (-0.86), and E_G is the band gap of the material (418 meV). The fit is excellent for most samples, although it somewhat underestimates the masses for sample 1252 (a thin-layer sample which is strongly n-type), and overestimates the masses of the very wide-layer samples, such as 1266.

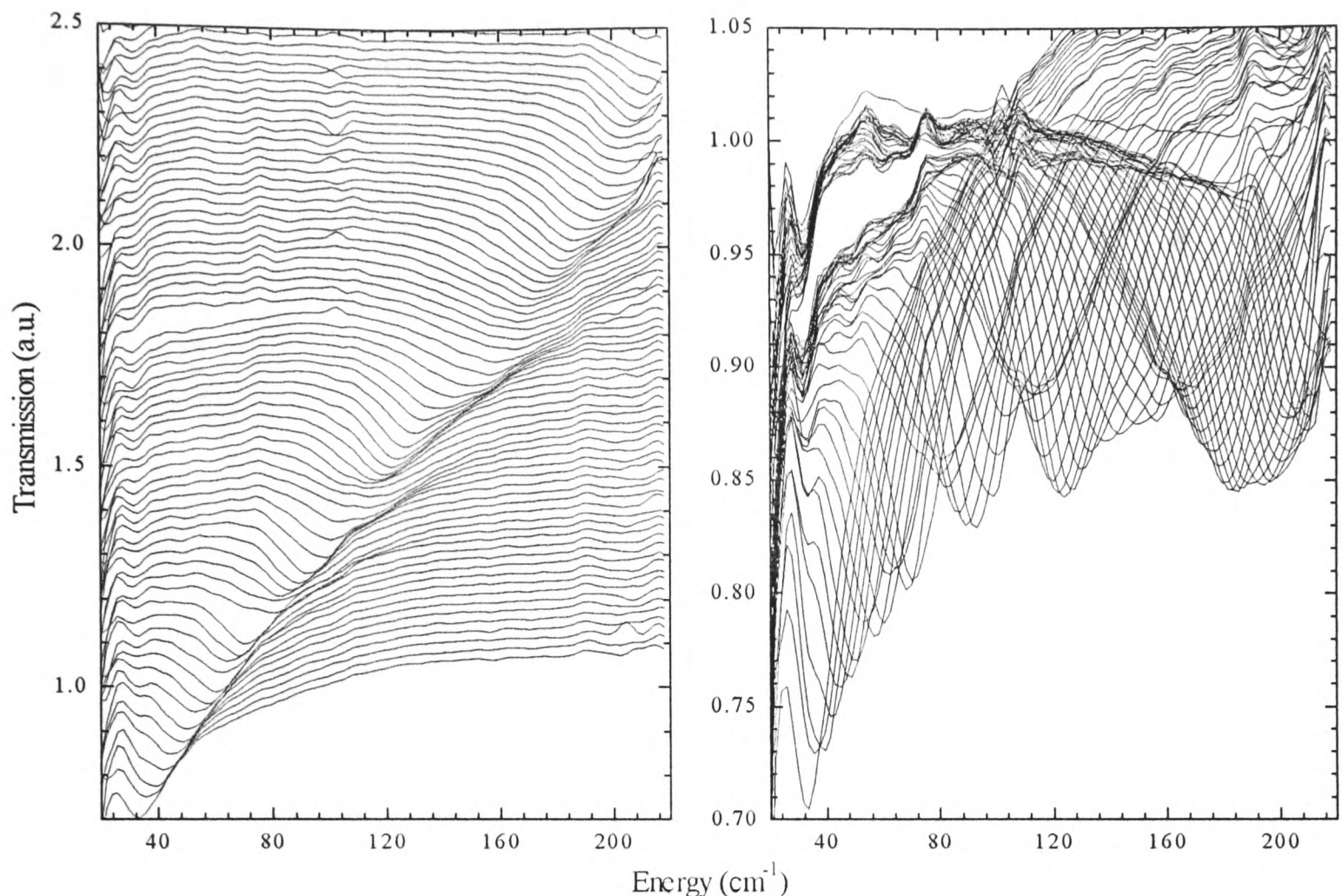


Figure 3.16: Two views of the cyclotron resonance data from sample 2105 [001]. The spectra start at the top at 8 T, and descend in 0.1 T steps to 1 T at the bottom (all ratioed against the 14 T trace). The plot on the left is offset, showing “ripples” as the linewidth and intensity oscillate. The plot on the right is the raw data, showing oscillations in the resonance intensity.

The kinetic energy of the electrons at the Fermi level $\langle T \rangle$ is computed as the kinetic energy of the bound state $\langle k_z^2 \rangle$ plus the energy from the bottom of the state to the Fermi level:

$$\langle T \rangle = \langle k_z^2 \rangle + (E_F - E_0) . \quad (3.11)$$

Fig. 3.15 shows reasonable agreement with experimental results.

As a result of these CR experiments, the electron effective mass is observed to be dependent on the InAs layer thickness, a direct consequence of the confinement energy variation with well width. The apparent weak dependence of mass on orientation and indium concentration is likewise an artifact of confinement effects.

3.7 Oscillations in Linewidth and Intensity

CR of double heterojunctions (DHETs) behaves slightly different from superlattice CR. There are much fewer carriers, so the absorption tends to be weaker. DHETs are much more strongly n-type, so that hole resonances are rarely observed. The most important difference,

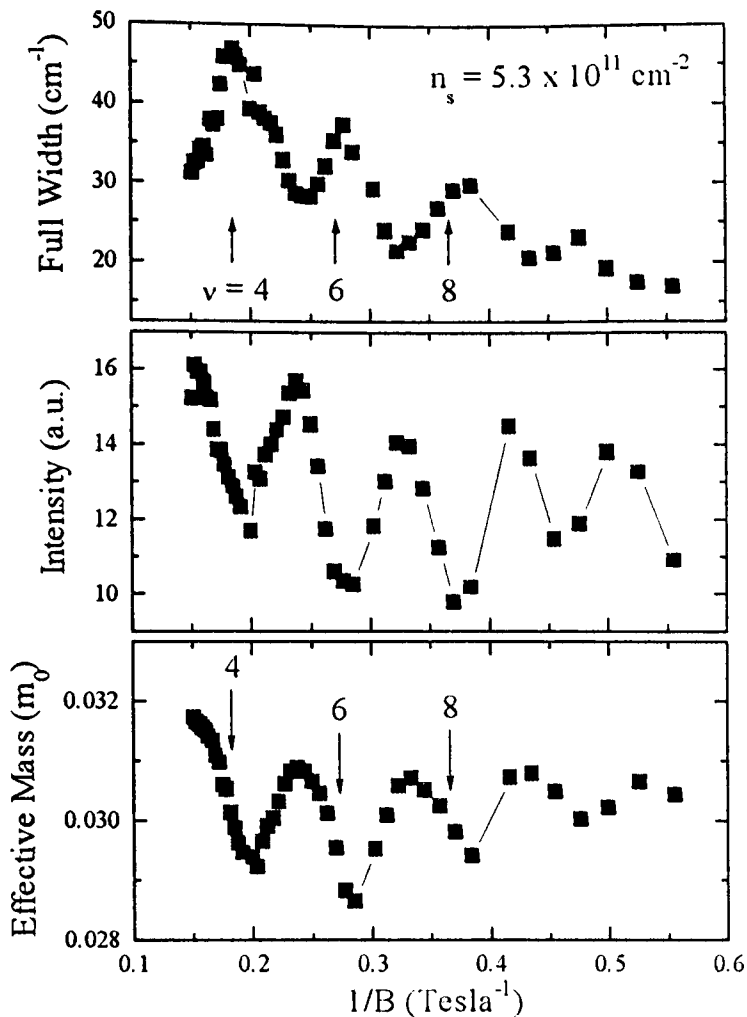


Figure 3.17: Observed oscillations in sample 2105 [001], with the deduced carrier density.

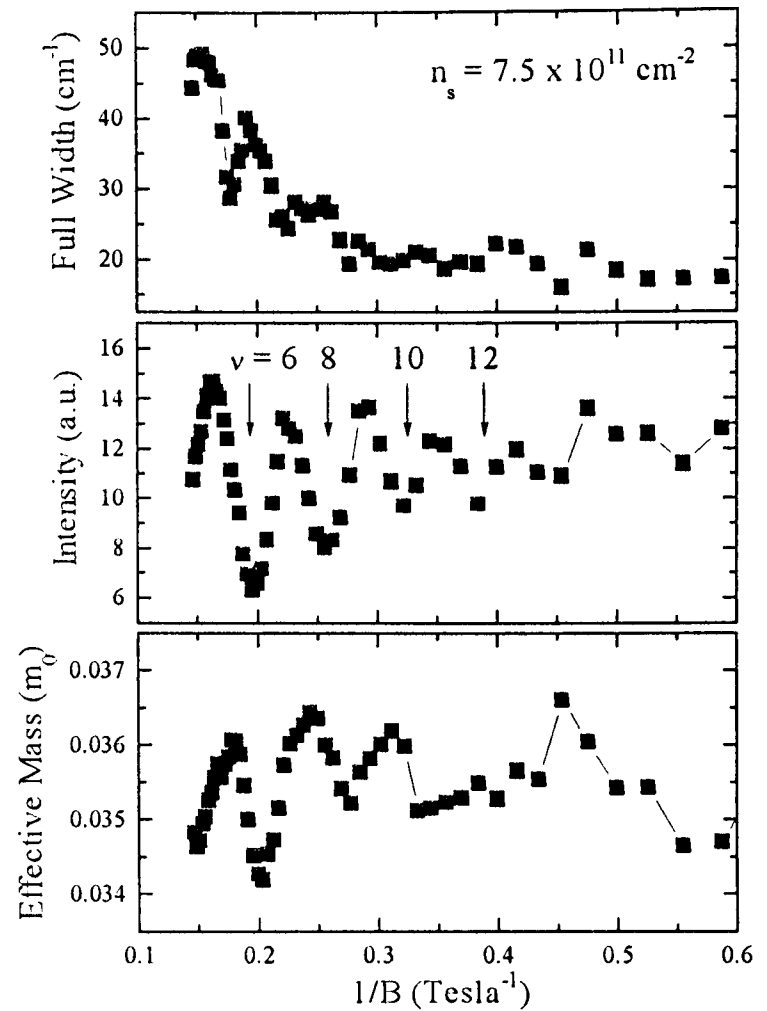


Figure 3.18: Observed oscillations in sample 1179 [001], with the deduced carrier density.

however, is that oscillations are observed in the resonance position, intensity, and linewidth. The raw data for one high-quality heterojunction, sample 2105 [001], is presented in Fig. 3.16.

The oscillations are related to the filling factor ν , and jumps in the resonance position, linewidth and intensity are observed when Landau levels cross the Fermi level. Owing to the linear nature of the Landau level energies with field, the oscillations are periodic in $1/B$. One can deduce the carrier density n_s of the sample by looking at the period η (in units of $1/B$) of the oscillations, via the equation

$$n_s = \frac{e}{2 h c \eta}, \quad (3.12)$$

where it is assumed that the oscillations are not spin-resolved. The oscillatory features and deduced carrier density for samples 2105 [001] and 1179 [001] are given in Figs. 3.17 and 3.18. The carrier density derived for 2105 [001] is within 10% of that determined by transport measurements [29] (no transport has been performed on 1179 [001]).

Originally, CR oscillations in InAs were thought to arise from the filling-factor-dependent screening of impurities in the heterostructure [18]. However, no explanation was

developed as to why the screening effect should be so much more pronounced in InAs than GaAs. Later experiments also refuted the screening argument.

Hansen *et al.* [30] showed via a two-band Kane model that nonparabolicity would induce filling-factor-dependent oscillations in 2D CR. However, the nonparabolicity argument predicts linewidth minima and intensity maxima at even filling factors, inconsistent with our results (see Figs. 3.17 and 3.18). CR oscillations of electrons in InAs wells with AlSb barriers *are* consistent with the nonparabolicity results [20,19]. It is therefore puzzling that the nature of the barrier should so completely determine whether the InAs electrons oscillate due to nonparabolicity or screening effects.

Kono *et al.* [21] performed CR on InAs/(Al,Ga)Sb heterojunctions. Samples with a low Al content (10-20%) exhibited resonance oscillations similar to ours, *e.g.*, the opposite expected for nonparabolicity effects. Samples with larger Al content showed no evidence of oscillations. They note that, given the similarity of the 2D systems mentioned above, the only variable which can account for the unusual behavior of InAs/GaSb oscillations is the coexistence of electron and hole populations. The Kono data was particularly conclusive, as the low Al content samples (which showed oscillations) were semimetallic, whereas samples with 30% or more Al (which showed no oscillations) were semiconducting by nature of the conduction and valence band lineups.

Kono *et al.* give no clear mechanism for the oscillations. In their samples they also see an “X” resonance which sits $20\text{-}30\text{ cm}^{-1}$ above the cyclotron transition. They assign the X line to an internal transition of electron-hole excitons. Their data indicates a filling factor dependence of the X line, and so implicitly a filling-factor-dependent electron-hole interaction. This interaction, they claim, is the most likely source of the oscillations.

Warburton *et al.* [10] also observe resonance oscillations related to the electron filling factor in their InAs quantum well. In one p-type sample, where both electrons and holes are present, they observe strong low-field spin-splitting of the electron line as well as oscillations in linewidth, intensity, and effective mass. The oscillations match those observed by Kono [21] and the Clarendon samples presented here. Their n-type sample, with no holes, exhibits neither spin-splitting or oscillations.

No X line or low-field spin-splitting was observed in any of our heterojunctions, yet all display some degree of resonance oscillation, and all are inconsistent with the conventional extrinsic nonparabolicity argument. The above-mentioned experimental data compels one to

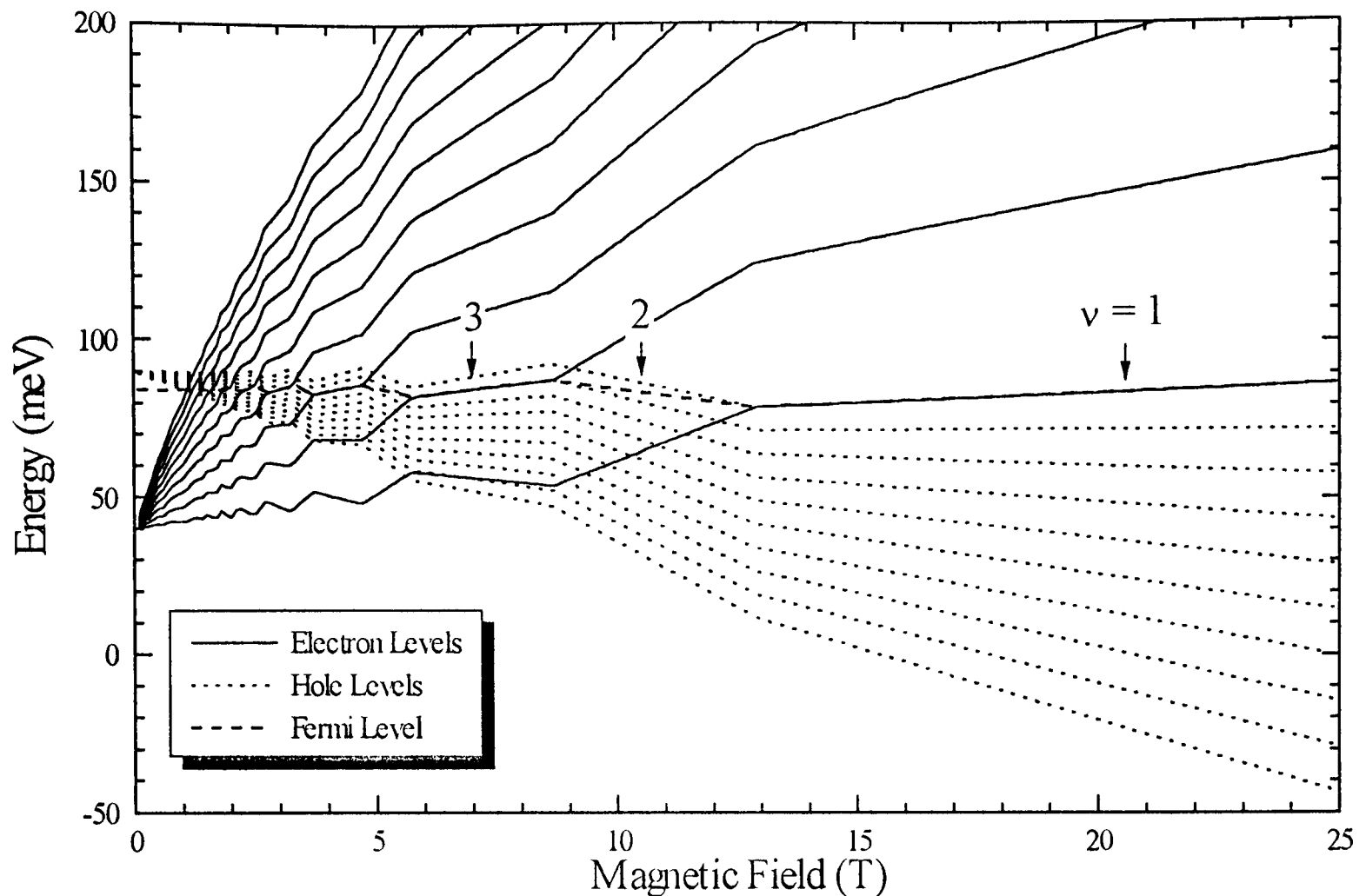


Figure 3.19: Landau levels of a simple spin-degenerate electron-hole system, with a nonparabolic electron effective mass (details given in Chapter 7). The filling factors are given for a density of $5 \cdot 10^{11} \text{ cm}^{-2}$, although the density varies with field (see Fig. 3.20). Note the coincidence of the electron and hole levels at the Fermi level for odd filling factors.

agree that the coexistence of electron and hole populations must be at the heart of the oscillations.

There is one spectacular difference between this intrinsic system and other n- or p-type systems: electron and hole Landau levels *must* cross the Fermi level at the same time. This means that at odd filling factors, electron and hole levels coexist at the Fermi level of the system. At even filling factors, the Fermi level lies between the highest populated electron and lowest populated hole levels. Landau levels from a simple self-consistent model (explained in Chapter 7) are displayed in Fig. 3.19. In the region of odd filling factors, the levels are depopulating with field. In the region of even filling factors, the levels are repopulating with field. This will give the carrier density, and so the Coulombic potential, an oscillatory behavior which depends on filling factor.

For a nominally constant Fermi level, nonparabolicity will cause the effective mass to oscillate with field (see Fig. 3.20). The effective mass is expected to be a minimum just past even filling factors, and a maximum past odd filling factors (thermal distribution of carriers, not considered in this model, will smooth out the sawtooth shape of Fig. 3.20). One interesting result is that the maxima in the oscillations occur at fractional filling factors. This

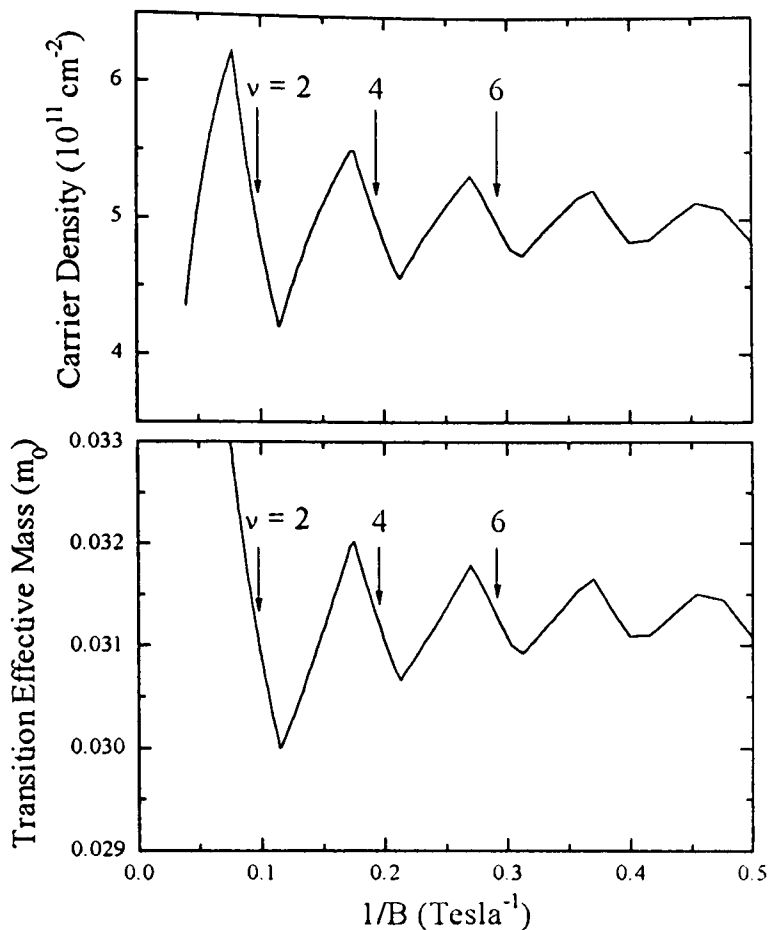


Figure 3.20: Oscillations in carrier density and transition effective mass as calculated from the Landau levels in Fig. 3.19.

It should be emphasized that the theory of Hansen *et al.* [30] considered constant (extrinsic) carrier densities, such that as a Landau level depopulated, a new cyclotron transition with different mass was available. In our intrinsic case, depopulation of a Landau level actually reduces the carrier density in the whole structure, and it is these total density oscillations which dominate the nonparabolicity effects.

Nicholas *et al.* [31] have shown that oscillations in effective mass (or resonance position) lead directly to oscillations in the linewidth. They use a modified Kramers-Kronig analysis to find

$$\Gamma(B) = -\frac{1}{\pi} \int \frac{\Delta(B') dB'}{B' - B}, \quad (3.13)$$

where $\Gamma(B)$ is the broadening (linewidth), and $\Delta(B)$ is the shift in resonance position due to oscillations in the effective mass. The integration ensures that oscillations in linewidth will be out of phase with oscillations in effective mass, in agreement with experiments (see Figs. 1.19 and 1.21). The model therefore predicts that resonance linewidths should be a maximum at even filling factors.

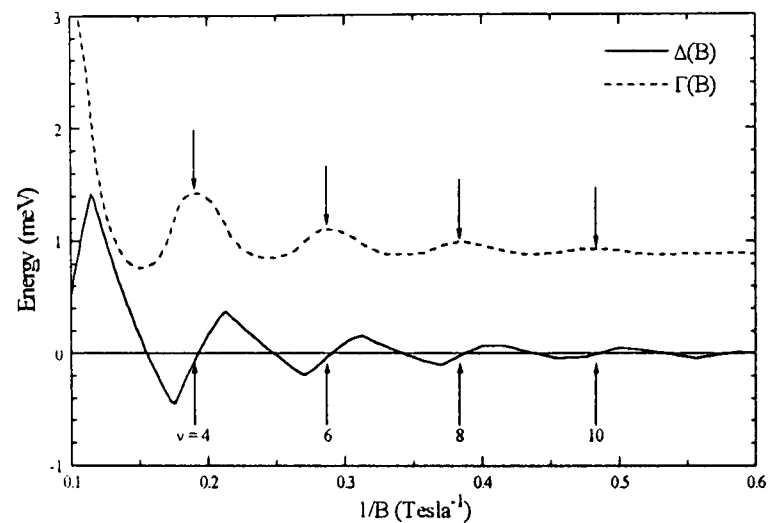


Figure 3.21: Resonance shift $\Delta(B)$ and broadening $\Gamma(B)$ as a function of filling factor, as calculated from Fig. 3.20 and Eq. (3.13).

model therefore provides a simple mechanism whereby nonparabolicity, along with the coexistence of large electron and hole populations, explains the effective mass oscillations observed.

To conclude, CR measurements on InAs/GaSb DHETs exhibit oscillations in linewidth, intensity, and effective mass. These results match other experiments in InAs/GaSb systems [10,18,21], with oscillations that are opposite in nature to those observed in InAs/AlSb systems [20,19]. These oscillations cannot be explained by nonparabolicity effects, nor can screening arguments explain the differences between GaSb and AlSb barrier systems. It has been proposed [21] that some sort of electron-hole interaction is responsible. It is shown here that oscillations in the effective mass are a direct result of nonparabolicity in a two-carrier system, and this leads via a simple Kramers-Kronig transformation to linewidth and intensity oscillations.

3.8 Conclusions

In this chapter, CR was used to examine three phenomena. First, a study of the heavy hole effective masses showed pronounced anisotropy with growth direction, which was shown to originate from the anisotropy of bulk GaSb. The effects of quantum confinement plus the large nonparabolicity of InAs explained the observed electron effective mass dependence on InAs layer width. Finally, measurements of InAs/GaSb double heterojunctions showed oscillations in resonance intensity, linewidth, and mass. These oscillations are almost certainly due to the unique intrinsic nature of the InAs/GaSb system, and mechanisms were proposed to explain the oscillations.

3.9 References

- [1] Fletcher, Yager, and Merritt, *Phys. Rev.* **100** (1955) 747.
- [2] G. Dresselhaus, A. F. Kip, and C. Kittel, *Phys. Rev.* **92** (1953) 827; G. Dresselhaus, A. F. Kip, and C. Kittel, *Phys. Rev.* **98** (1955) 368.
- [3] G. M. Summers, *D. Phil. Thesis*, Clarendon Laboratory, Oxford 1993.
- [4] J. G. Michels, *D. Phil. Thesis*, Clarendon Laboratory, Oxford 1994.
- [5] M. Lakrimi, T. A. Vaughan, R. J. Nicholas, D. M. Symons, N. J. Mason, and P. J. Walker, *Solid State Elect.* **37** (1994) 1227.
- [6] H. L. Stormer, Z. Schlesinger, A. Chang, D. C. Tsui, A. C. Gossard, and W. Wiegmann, *Phys. Rev. Lett.* **51** (1983) 126.
- [7] T. Ando, *J. of the Phys. Soc. of Japan* **54** (1985) 1528.
- [8] U. Ekenberg and M. Altarelli, *Phys. Rev. B* **32** (1985) 3712.

- [9] J. Luo, H. Munekata, F. F. Fang, and P. J. Stiles, *Phys. Rev. B* **41** (1990) 7685.
- [10] R. J. Warburton, B. Brar, C. Gauer, A. Wixforth, J. P. Kotthaus, and H. Kroemer, in *Proceedings of the 8th Conference on Modulated Semiconductor Structures*, to be published in *Solid State Elect.* (1995).
- [11] D. M. Symons, *D. Phil. Thesis*, Clarendon Laboratory, Oxford 1994.
- [12] Landolt-Börnstein, *Numerical Data and Functional Relationships in Science and Technology*, New Series Group III vol. 17a, edited by O. Madelung, Springer-Verlag, Berlin, 1982, pp. 258-278, 297-310.
- [13] H. Sakaki, L. L. Chang, G. A. Sai-Halasz, C. A. Chang, and L. Esaki, *Solid State Comm.* **26** (1978) 589.
- [14] H. Bluysen, J. C. Maan, P. Wyder, L. L. Chang, and L. Esaki, *Solid State Comm.* **31** (1979) 35; H. J. A. Bluysen, J. C. Maan, P. Wyder, L. L. Chang, and L. Esaki, *Phys. Rev. B* **25** (1982) 5364.
- [15] Y. Guldner, J. P. Vieren, P. Voisin, M. Voos, L. L. Chang, and L. Esaki, *Phys. Rev. Lett.* **45** (1980) 1719; Y. Guldner, J. P. Vieren, P. Voisin, M. Voos, J. C. Maan, L. L. Chang, and L. Esaki, *Solid State Comm.* **41** (1982) 755.
- [16] J. C. Maan, Y. Guldner, J. P. Vieren, P. Voisin, M. Voos, L. L. Chang, and L. Esaki, *Solid State Comm.* **39** (1981) 683.
- [17] R. A. Stradling, *Phys. Lett.* **20** (1966) 217.
- [18] D. Heitmann, M. Ziesmann, and L. L. Chang, *Phys. Rev. B* **34** (1986) 7463.
- [19] M. J. Yang, R. J. Wagner, B. V. Shanabrook, J. R. Waterman, and W. J. Moore, *Phys. Rev. B* **47** (1993) 6807.
- [20] J. Scriba, A. Wixforth, J. P. Kotthaus, C. R. Bolognesi, C. Nguyen, G. Tuttle, J. H. English, and H. Kroemer, *Semicond. Sci. Tech.* **8** (1993) S133.
- [21] J. Kono, B. D. McCombe, J.-P. Cheng, I. Lo, W. C. Mitchel, and C. E. Stutz, *Phys. Rev. B* **50** (1994) 12242.
- [22] L. S. Kim, H. D. Drew, H. Munekata, L. L. Chang, and L. Esaki, *Solid State Comm.* **66** (1988) 873.
- [23] G. M. Sundaram, R. J. Warburton, R. J. Nicholas, G. M. Summers, N. J. Mason, and P. J. Walker, *Semicond. Sci. Tech.* **7** (1992) 985.
- [24] C. Weisbuch and B. Vinter, *Quantum Semiconductor Structures: Fundamentals and Applications*, Academic Press, London, 1991.

- [25] R. J. Warburton, R. A. Lewis, R. J. Nicholas, N. J. Mason, and P. J. Walker, *Physica B* **184** (1993) 154.
- [26] A. P. Roth and E. Fortin, *Can. J. Phys.* **56** (1978) 1468.
- [27] R. A. Morrow and K. R. Brownstein, *Phys. Rev. B* **30** (1984) 678.
- [28] E. D. Palik, G. S. Picus, S. Teitler, and R. F. Wallis, *Phys. Rev.* **122** (1961) 475.
- [29] M. Lakrimi, private communication.
- [30] E. B. Hansen and O. P. Hansen, *Solid State Comm.* **66** (1988) 1181.
- [31] R. J. Nicholas, M. A. Hopkins, D. J. Barnes, M. A. Brummell, H. Sigg, D. Heitmann, K. Ensslin, J. J. Harris, C. T. Foxon, and G. Weimann, *Phys. Rev. B* **39** (1989) 10955.

Chapter 4

Saturated Cyclotron Resonance

This chapter concerns cyclotron resonance experiments performed at the picosecond pulsed free electron laser at FELIX, in Rijnhuizen, the Netherlands. The use of a free electron laser allowed for peak laser intensities approaching 1 MW/cm^2 . With these high intensities, the absorption process saturates, and information about the Landau level lifetimes may be extracted as a result. When the wavelength-dependence of the lifetimes is studied, strong evidence for the resonant emission of phonons is found.

4.1 INTRODUCTION	77
4.2 EXPERIMENTAL SETUP	78
4.3 THE FREE ELECTRON LASER	78
4.4 THEORY	81
4.5 RESULTS AND DISCUSSION	85
4.6 CONCLUSION.....	88
4.7 REFERENCES	89

4.1 Introduction

Cyclotron resonance (CR) saturation spectroscopy has been used to determine carrier lifetimes in bulk materials for several decades [1,2], and is now being applied to heterostructures as well [3,4,5]. By saturating the absorption process in magnetic fields, the lifetimes of the Landau levels may be determined. The motivation for these studies is understanding of the relaxation mechanisms in InAs/GaSb heterostructures, as device performance will depend on the relevant lifetimes of states.

Saturation [1,2] and time-resolved optical studies [6-10] on bulk structures reveal three general mechanisms of non-radiative relaxation. For low density structures with carriers in energy levels below the optical phonons, acoustic phonon scattering is the dominant relaxation mechanism, with lifetimes on the order of 10 ns, with little density dependence. Structures with moderate to high carrier densities occupying states below the optical phonons thermalize via carrier-carrier scattering, with density-dependent lifetimes on the order of 1 ns. Any carriers in higher states can relax via optical phonon scattering with lifetimes on the order of 1 ps, with some density dependence. The distinction between different mechanisms is somewhat blurred, as high-density systems can have carrier-carrier scattering lifetimes on the order of 10 ps, close to the LO-phonon lifetime [4]. Likewise, interband excitation places electrons far up the conduction band, electrons which then cascade down and can saturate the LO-phonon population, leading to long LO-phonon relaxation lifetimes of 10-30 ps [7,8]. Previous CR saturation studies of 2D systems [4,5] have been performed on moderate-density samples with carriers occupying states below the optical phonon band, and so saw only carrier-carrier scattering with nanosecond lifetimes.

If carriers have access to LO-phonons, oscillatory features in magnetic fields may arise as a result of the magnetophonon effect (resonant absorption or emission of LO-phonons), which occurs when the energy separation between two Landau states is equal to the bulk LO-phonon energy, *i.e.*,

$$N \hbar \omega_c = \hbar \omega_{LO} , \quad (4.1)$$

for some integer N , where $\hbar \omega_c$ is the CR transition energy, and $\hbar \omega_{LO}$ is the optical phonon energy [12]. The magnetophonon effect in 2D GaAs/AlGaAs systems has been extensively

investigated. Barnes *et al.* [13] observed magnetophonon resonances (MPR) in the linewidth of CR, a direct observation of oscillations in the momentum relaxation time. Hot-electron MPR has been indirectly observed in magnetoresistance [14,15], and directly observed in phonon measurement studies [16].

This study is unique in several ways: it is the first saturated CR experiment to see Landau level lifetimes as short as a picosecond, it is the first experiment to observe the MPR effect in the InAs/GaSb system, and it is the first experiment in any 2D system to observe oscillations in level lifetime due to resonant phonon emission.

4.2 Experimental Setup

The sample studied is an InAs/GaSb double heterojunction, grown by MOVPE on a GaAs undoped substrate (see Chapter 1 and the references therein). A thick GaSb buffer layer ($\sim 1\ \mu\text{m}$) is grown on top of the substrate to accommodate strain, then a thin-layer semiconducting InAs/GaSb superlattice, followed by the 400 Å InAs layer, and finished with a 200 Å GaSb capping layer. The carrier density at helium temperatures has been determined by transport measurements to be $6.0 \times 10^{11}\ \text{cm}^{-2}$, with a mobility of $40,000\ \text{cm}^2/\text{Vs}$. Transport measurements and self-consistent calculations (performed in the effective mass approximation as described in Chapters 2 and 3) indicate that one electron state and one heavy hole state are occupied. The substrate of the sample was wedged to avoid interference effects, however the substrate prevented us from measuring in the GaAs reststrahlen band (31-37 meV).

The sample was mounted in the Faraday configuration (light and magnetic field normally incident to the sample) in a superconducting magnet. The laser was directed to the sample via a light pipe and focused on the surface with a cone, calibrated attenuators being used to vary the laser intensity. The transmission was measured by a thinned Allen-Bradley resistor mounted behind the sample in the cryostat, with a second resistor mounted in front of the sample in the light pipe as a reference. The sample and detectors were cooled to 2K.

4.3 The Free Electron Laser

The measurements were performed using the far infrared picosecond free electron laser FELIX at Rijnhuizen [17]. As the name suggests, in a free electron laser it is free electrons which lase, rather than electrons bound in atoms, molecules, or crystals. The basic principle is that relativistic electrons are injected into an “undulator,” a periodic array of magnetic fields. The alternating form of the magnetic field leads to an oscillating electron trajectory, with

dipole radiation being emitted. Although this dipole radiation is essentially incoherent, placing mirrors at each end of the undulator chamber (with the electron path bent so that the electrons themselves never contact the mirrors) results in a laser cavity, with resonant amplification of certain wavelengths depending on the electron beam energy and spacing between magnets. These two parameters, the beam energy and magnet spacing, can be modified in minutes, allowing relatively quick and precise variation of the laser wavelength.

The electron pulse in FELIX is created by a thermionic triode electron gun, modulated at 1 GHz with typically 5 pulses per second, each pulse being 3-6 μs long. The pulse is then fed through a radio-frequency linear accelerator (r.f. linac), which injects the now relativistic electrons into the undulator chamber. Due to the pulse characteristics of the electron gun and r.f. linac, the output of FELIX consists of 5 “macropulses” per second, each macropulse consisting of a number of “micropulses.” Each micropulse of the laser is typically several ps long, separated by 1 ns. There are two undulator chambers at FELIX, one for operation in the wavelength range of 16-110 μm , and the other for shorter wavelengths of 5-30 μm . In these experiments, wavelengths of 30-105 μm (photon energies of 12-40 meV) were required, so the long-wavelength undulator was used.

A standard thermocouple power meter is used to measure the average power of the laser. It is therefore necessary to extract the peak intensity of each micropulse from this average power measurement. To do so requires some knowledge of the pulse structure. A gaussian intensity distribution of

$$I(t) \propto \exp[- 1/2 (t / \sigma_t)^2], \quad (4.2)$$

when Fourier-transformed, results in a power spectrum

$$P(\omega) \propto \exp[- 1/2 (2 \sigma_t \omega)^2], \quad (4.3)$$

where σ_t is a parameter describing the width of the pulse. Although the power spectrum of FELIX is not given, the spectral width (full width at half-maximum, FWHM) of the laser $\Delta\lambda$ is known from real-time spectral analysis at one of FELIX’s diagnostic stations. The FWHM of the power spectrum $\Delta\omega$ can then be calculated using the identity

$$\omega = \frac{2 \pi c}{\lambda} \Rightarrow \Delta\omega = \frac{2 \pi c}{\lambda} \frac{\Delta\lambda}{\lambda}. \quad (4.4)$$

Fourier-transforming the power spectrum back and integrating over the entire pulse gives the total energy per micropulse

$$E_{pulse} = 2 P_0 \sqrt{\frac{\ln 2}{\pi}} \frac{\lambda}{c} \frac{\Delta\lambda}{\lambda}, \quad (4.5)$$

where P_0 is the peak power in the micropulse. From the spectral width $\Delta\omega$ the FWHM of the intensity in the micropulse Δt_μ can also be calculated, as

$$\Delta t_\mu = 2 \ln 2 \frac{\lambda}{\pi c} \frac{\lambda}{\Delta\lambda}, \quad (4.6)$$

which given typical values of $\Delta\lambda/\lambda \approx 1\%$, results in micropulse widths of $\Delta t_\mu \approx 8$ -12 ps for our experiment.

The total incident laser energy per second is then the energy per pulse of Eq. (4.5) multiplied by N , the total number of pulses per second. This is given as $N = \Delta t_M f_M f_\mu$, where Δt_M is the macropulse FWHM (3-6 μ s), f_M is the macropulse frequency (5 Hz), and f_μ is the micropulse frequency (1 GHz). This results in the total (average) power per second $P = N E_{pulse}$. The average power is multiplied by the transmission of the light pipe T , and divided by the area illuminated on the sample to arrive at an expression relating the peak intensity I and the measured average power:

$$I = \frac{1}{2} \frac{P T}{\sqrt{\pi \ln 2}} \frac{1}{r^2} \frac{c}{\lambda} \frac{\Delta\lambda}{\lambda} [\Delta t_M f_M f_\mu]^{-1}, \quad (4.7)$$

where r is the radius of the illuminated spot on the sample. For these experiments, T was measured to be around 0.1, and r was taken to be the radius of the cone aperture (0.75 mm).

For each measurement, the wavelength λ was established. The widths $\Delta\lambda$ and Δt_M were read from spectral analysis of the laser, and the average power P was measured with a power meter. The frequencies f_M and f_μ and the aperture r were constant for all measurements

(T was assumed to be wavelength-independent as well), and so the peak intensity I could be readily calculated from Eq. (4.7). The greatest uncertainty is the transmission of the light pipe, or more precisely, the measurement of how much power is lost as the laser makes its way through the room-temperature optics, then down through the insert to the sample. Care was taken to avoid strong water absorption, and the transmission of the light pipe was measured, but the value of T (and so the peak intensity I) is probably only accurate to within a factor of two.

4.4 Theory

The absorption process in a multi-level system is saturated by having an incident photon flux (intensity) so large that all available levels in the system are populated, with resonant absorption and stimulated emission between levels closely matched so that no net absorption occurs. Saturation of CR therefore requires that the equidistant ladder of Landau levels be truncated at some point, as otherwise increasing intensity merely results in higher states being populated. In low density GaAs/AlGaAs heterostructures the polaron effect is used, where coupling with the LO-phonon band alters the Landau level structure. In high density samples ($n_s \geq 4 \times 10^{11} \text{ cm}^{-2}$) the polaron effect is suppressed, and in the GaAs/AlGaAs system this means that saturation is difficult to achieve.

The polaron effect is likewise suppressed for our density of $6.0 \times 10^{11} \text{ cm}^{-2}$, but saturation is still possible due to the nonparabolicity of the Landau states. InAs has a relatively small band gap (418 meV), hence the nonparabolicity of the conduction band mass is much larger than in GaAs (with a band gap of 1520 meV). The nonparabolicity of the effective mass is written as a function of the observed transition energy $\hbar\omega_c$ as [18]

$$m^*(E) = m_0^* [1 + (2.6 (n+1) \hbar\omega_c + E_{conf}) / E_G], \quad (4.8)$$

where m_0^* is the band-edge effective mass ($m_0^* = 0.023 m_0$ in InAs), E_G is the band gap, E_{conf} the bound state energy due to quantum confinement in the growth direction, and $\hbar\omega_c$ the transition energy between the n and $n+1$ Landau levels. A value of $E_{conf} = 47 \text{ meV}$ is found to best fit the observed low-intensity transitions, which is in good agreement with self-consistent calculations.

The high carrier density does not allow for simple analysis of the lifetimes. We are well below the quantum limit, and so have to take account of several fully or partially occupied Landau levels. For each level n , a rate equation accounting for stimulated emission, stimulated absorption and non-radiative emission is written as

$$\frac{df_n}{dt} = \Phi [A_{n-1} - A_n] - [f_n (1 - f_{n-1}) / \tau_n] + [f_{n+1} (1 - f_n) / \tau_{n+1}], \quad (4.9)$$

where A_n is the absorption between levels n and $n+1$, $\Phi = I / (2 N \hbar \omega)$ is the photon flux per electron, I is the incident laser intensity, f_n is the filling factor, and τ_n is the non-radiative relaxation lifetime. The relaxation process will in general be quite complicated, involving broadening- and field-dependent electron-electron scattering and LO-phonon emission between non-adjacent levels, and so I make the simplifying assumption of allowing non-radiative decay between adjacent levels only, with a phenomenological lifetime $\tau_n = \tau$ for all n . Using linearly polarized light renders only half of the incident light CR-active, therefore the photon flux has been divided by two.

The absorption per level A_n and total transmission T are defined as

$$A_n = \frac{4 \sigma_n / \sigma_0}{(1 + \eta + \sigma_n / \sigma_0)^2}, \quad (4.10)$$

and

$$T = \frac{4 \eta}{(1 + \eta + \sum \sigma_n / \sigma_0)^2}, \quad (4.11)$$

where η is the index of refraction of the substrate (~ 3.3 for GaAs), $\sigma_0 = \epsilon_0 c$ is the conductivity of free space, and σ_n is the filling-factor-dependent conductivity given by

$$\sigma_n = (n+1) N (f_n - f_{n+1}) \frac{e^2 m^* \tau_{cr}}{m^{*2} + [\tau_{cr} (m^* \omega - e B)]^2}, \quad (4.12)$$

where N is the total carrier density, and τ_{cr} is the momentum relaxation lifetime given by

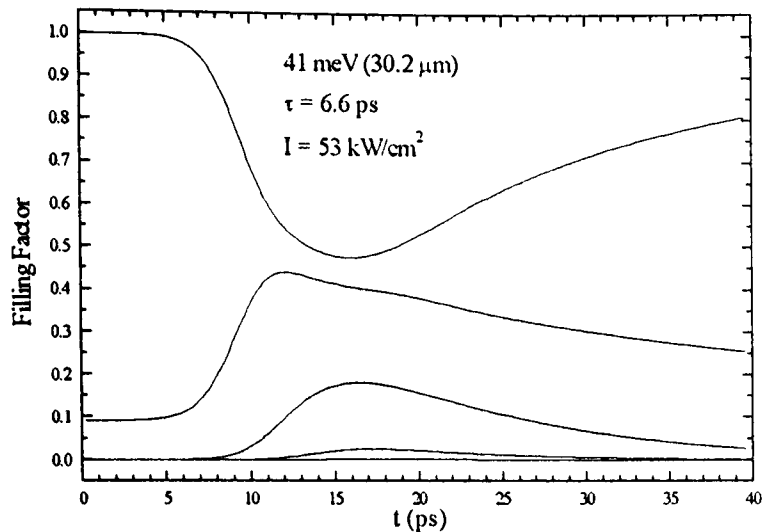


Figure 4.1: Filling factors of the various Landau levels throughout the micropulse for a photon energy of 41 meV.

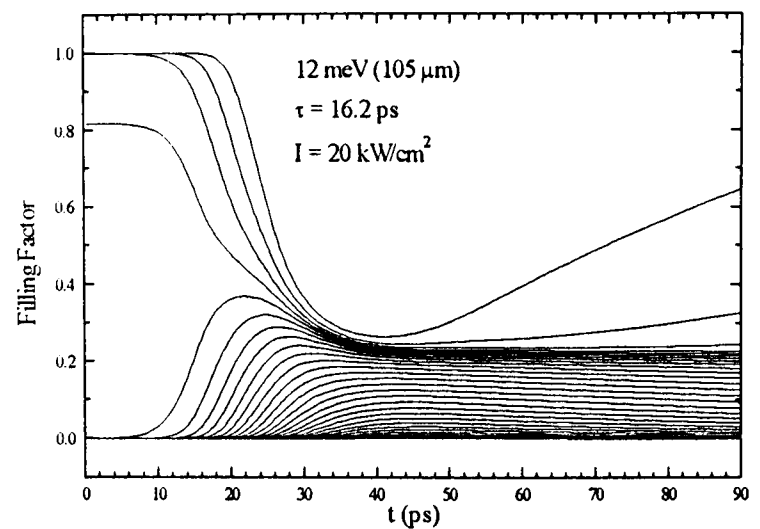


Figure 4.2: Filling factors of the various Landau levels throughout the micropulse for a photon energy of 12 meV.

$$\tau_{cr} = \frac{m^*}{e \Delta B}, \quad (4.13)$$

where ΔB is the HWHM of the resonance. The observed HWHM of $\Delta B \approx 0.6$ T corresponds to a lifetime of $\tau_{cr} \approx 0.3$ ps, consistent with the mobility. The details of the Landau ladder truncation are contained in Eq. (4.12): the effective mass m^* increases with the level index n (via Eq. (4.8)), so that the conductivities of higher-order Landau levels become negligible. At the saturation intensity (defined as the intensity at which the integrated absorption falls to one-half its low-intensity limit), only four levels are significantly populated at $\hbar\omega = 41$ meV, while twenty or more levels are populated for the low photon energies.

The set of coupled differential equations of Eq. (4.9) are solved numerically, with the total transmission integrated across the micropulse. The non-radiative relaxation lifetime τ is an input to the model, and so is fitted to reproduce the experimentally-observed saturation intensities. At all photon energies, the observed saturation intensities indicate lifetimes much shorter than the repetition rate of 1 ns, justifying the single micropulse model. The number of levels used in the calculation depends on the wavelength, in general levels were added until the lifetime changed by less than 0.01 ps.

Using the above analysis the Landau level lifetime τ may be determined as a function of photon energy and saturation intensity. The solutions to Eq. (4.9) are plotted in Figs. 4.1 and 4.2 for photon energies of 41 and 12 meV, respectively. At these energies, the saturation intensity is low, indicating a long relaxation lifetime. The model is not sensitive to lifetimes longer than micropulse (where little decay occurs during the pulse), so in these cases I use the

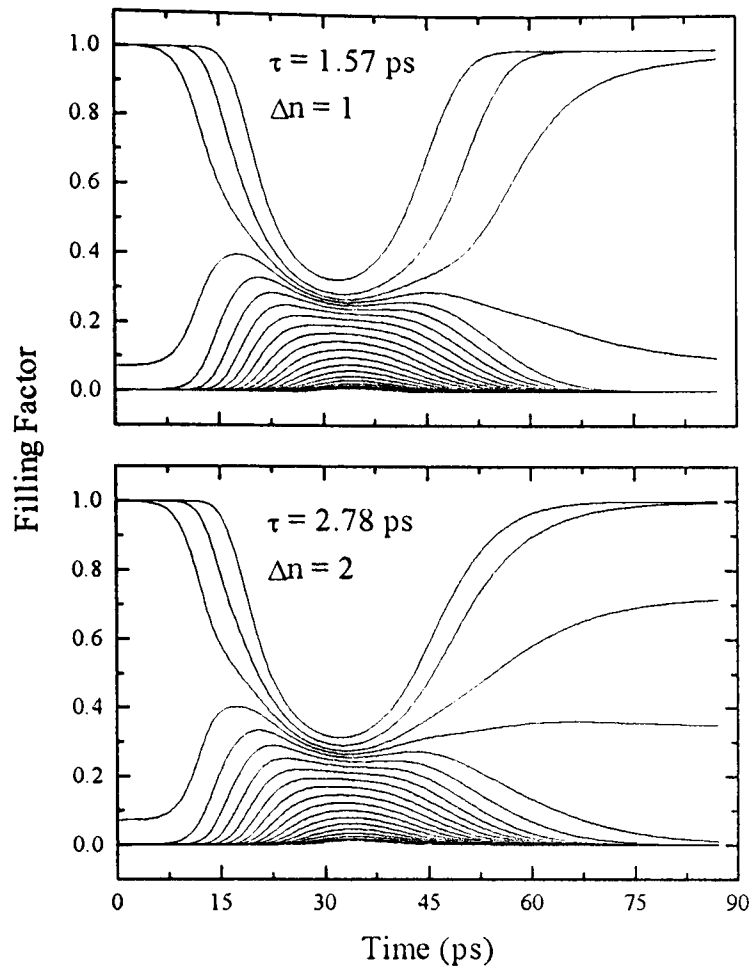


Figure 4.3: Filling factors for a photon energy of 15 meV (83.2 μm), at an incident intensity of 120 kW/cm². The top figure assumes that relaxation occurs between adjacent Landau levels, while in the bottom figure relaxation drops the electron down two levels at a time (the $N = 2$ MPR condition).

pulse full width as a lower bound on the lifetime. It is clear that a reduction in the photon energy (with a corresponding decrease in the resonance magnetic field) results in many more Landau levels being populated.

In Fig. 4.3, the population of each level is plotted at the saturation intensity as a function of time at the 14.9 meV laser energy ($2\omega_c = \omega_{LO}$), using the fitted level lifetimes. At $t = 0$ (just as the pulse turns on), three levels are fully populated, with a fourth level slightly populated. As the intensity increases with the onset of the micropulse, higher levels populate. Here the lifetime τ is short compared to the micropulse full width (14.6 ps in this case), so that decay occurs rapidly, unlike Figs. 4.1 and 4.2. For the case $\Delta n = 1$

(decay between adjacent levels), the populations return to their initial values as the pulse fades. For $\Delta n = 2$ (where the electron decays two levels at a time), the enhanced decay mechanism allows for a longer lifetime, but the populations do not return to their initial values. Instead, some carriers become “stranded” in higher levels, as the lowest levels are fully populated. Here the process of carrier-carrier scattering would return the populations back to their initial values, but on a longer timescale. Fitting the calculated populations at the peak of the

Table 4.1: Calculation and experimental parameters for each wavelength. At 14.90 meV the $\Delta n = 2$ lifetime is also included. Lifetimes marked with a dagger ($\dagger$) were determined to be longer than the pulse width, and so the value given is a lower limit.

Photon Energy $\hbar\omega$ (meV)	Resonance Field B (T)	Resonance HWHM ΔB (T)	Micropulse HWHM Δt_μ (ps)	Saturation Intensity I_s (kW/cm ²)	Fitted Lifetime τ (ps)	Number of Levels Included
11.81	3.25	0.58	8.1	40	16.2 [†]	30
14.90	4.04	0.58	7.3	120	1.57	20
					2.78 ($\Delta n=2$)	
17.71	4.98	0.52	9.0	47	6.61	15
22.70	6.70	0.67	4.4	47	8.8 [†]	10
24.80	7.10	0.61	4.6	128	1.38	8
30.10	8.45	0.67	8.9	230	0.85	8
41.06	11.36	0.61	3.3	53	6.6 [†]	5

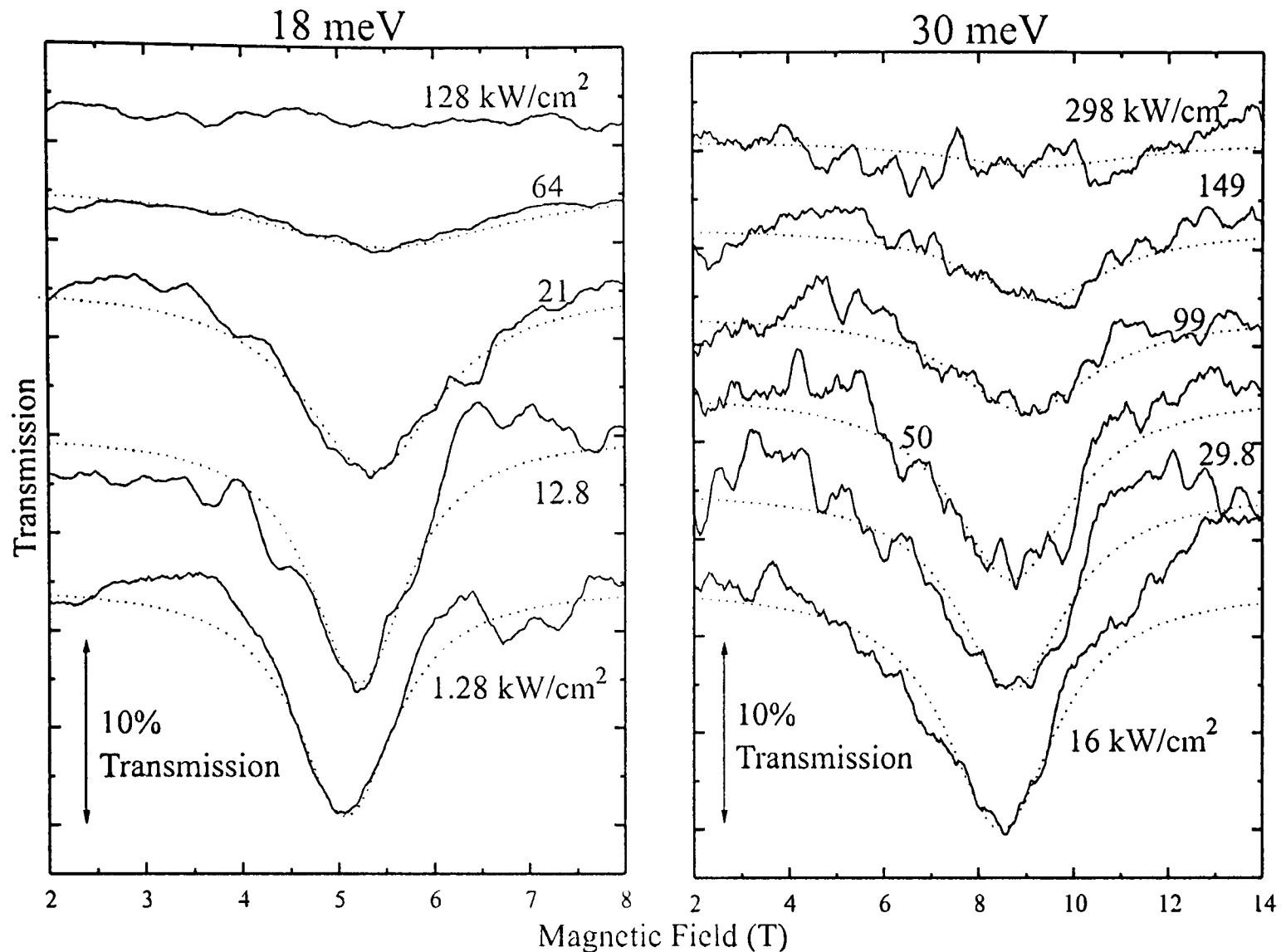


Figure 4.4: Transmission spectra at 18 and 30 meV, at several indicated laser intensities. The dashed lines are Lorentzian fits

micropulse to a Boltzmann distribution gives an electron temperature of roughly 500 K or more.

The model can be used to produce transmission versus magnetic field curves to fit the observed spectra. However, the model tends to result in spectra which are wider than the observed transitions at high intensities, due to transitions between higher states with higher effective masses. Lorentzians were therefore used to fit the data, as they were much faster and best able to reproduce the experimental lineshape.

4.5 Results and Discussion

Typical saturation spectra are presented in Fig. 4.4, as a function of power at laser energies of 18 and 30 meV. The LO phonon energy of InAs is also 30 meV, so here resonant polaron coupling would be expected to split the resonance into two branches. However it is known that the high carrier density used here causes a strong suppression of resonant polaron coupling due to the effects of level occupancy and no splitting is observed. As the intensity of the laser increases, the intensity of the absorption decreases, and the linewidth of the

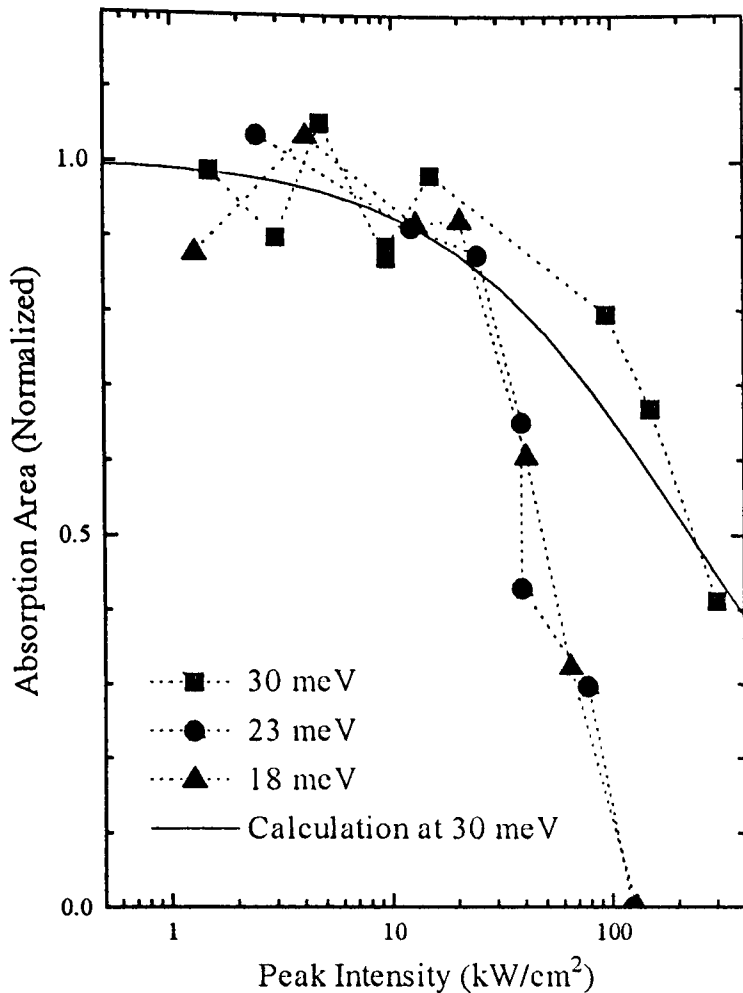


Figure 4.5: Integrated absorption area versus peak intensity, for a number of photon energies. The calculated area versus intensity is shown for the 30 meV energy.

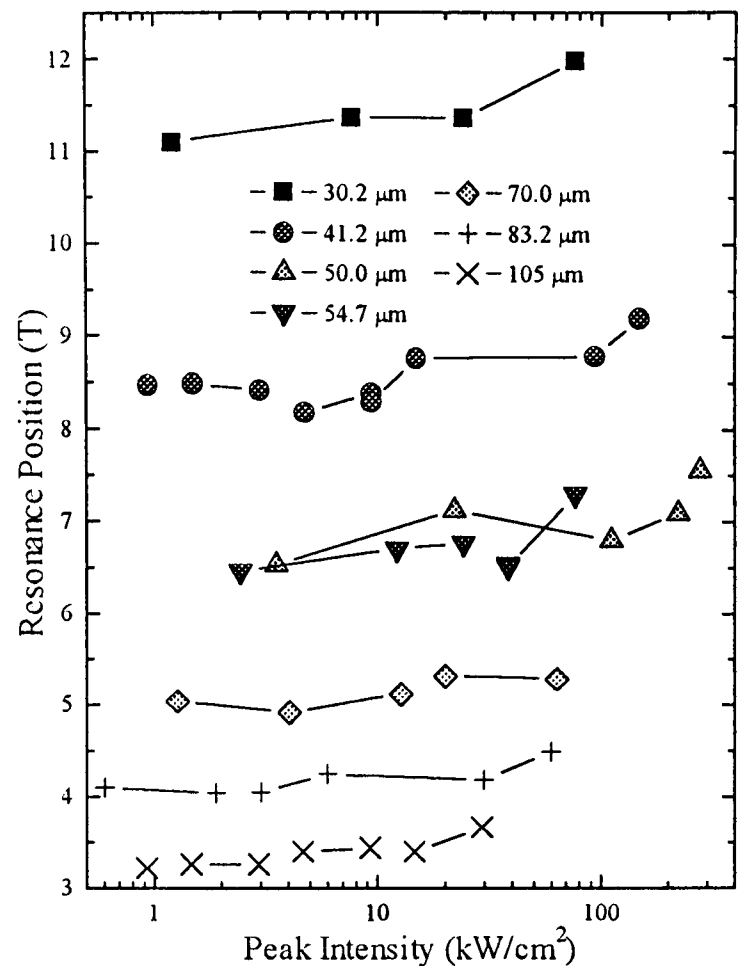


Figure 4.6: Resonance peak position as a function of peak laser intensity.

resonances increases. Care is taken to distinguish heating from saturation effects [5] by using the total integrated area of the resonance, since in the case of heating the area does not decrease with intensity, while the peak absorption still falls. The resonances were fitted with Lorentzian lineshapes. In Fig. 4.5 the area of the absorption resonances is plotted as a function of intensity for several wavelengths. The total area decreases in all cases, but the saturation behavior is clearly quite strongly dependent on the photon wavelength. The calculated saturation is also plotted for the 30 meV data.

In Fig. 4.6 the resonance position at each wavelength is plotted as a function of incident intensity. As the power is increased, the resonance shifts to higher fields, consistent with nonparabolicity effects. As electrons populate higher levels in the ladder, they sample a higher effective mass, which for a fixed wavelength shifts the resonance position to higher fields.

The saturation intensities and the fitted lifetimes are presented in Fig. 4.7. The intensities show clear peaks at the magneto-phonon resonance condition, leading to minima in the lifetimes there. The absolute accuracy of the lifetimes is relatively poor, due to systematic uncertainties in both the experimental parameters such as radiation intensity, which depends on

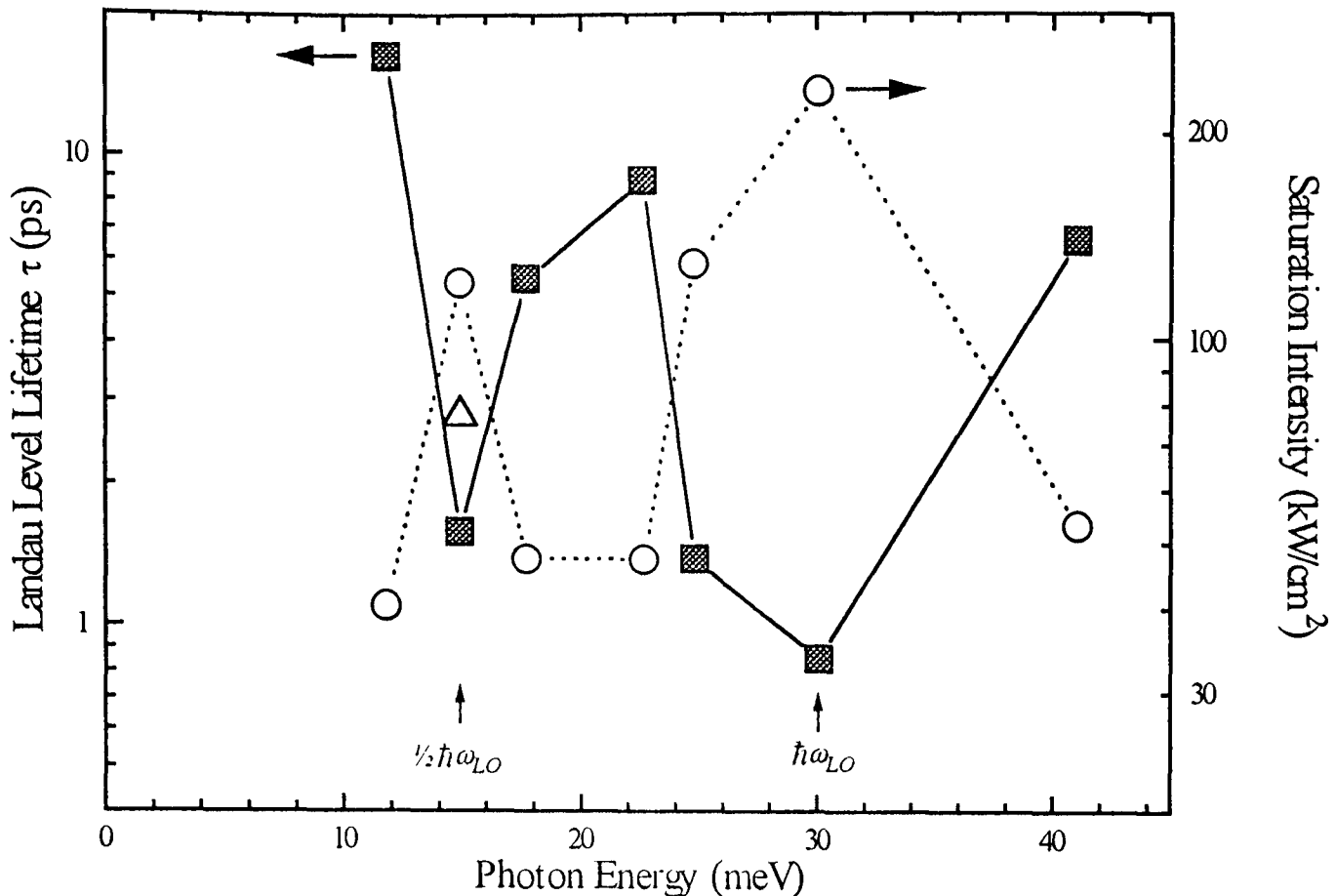


Figure 4.7: Saturation intensity and level lifetime as a function of photon energy. The lifetimes for 12, 23 and 41 meV are lower bounds, see text. The open triangle is the lifetime at 15 meV calculated for $\Delta n = 2$ (the $N = 2$ MPR condition of Eq. (4.1)).

the exact amount of focusing achieved in the cone arrangement above the sample and the transmission of the light pipe down the insert, and the assumptions used in the calculation. The absolute lifetimes are estimated to be accurate to within a factor of three. The relative accuracy is considerably better, of order $\pm 20\%$, since all measurements are made with a fixed experimental set-up, and use the same assumptions in the calculation.

Since LO phonon emission is a mono-energetic process, a detailed model would require non-radiative transitions with $\Delta n = 2$ for the $N = 2$ resonance of Eq. (4.1). A lifetime was calculated with this assumption at $2\omega_c = \omega_{LO}$, which although 75% longer than the $\omega_c = \omega_{LO}$ lifetime, is still considerably shorter than lifetimes at nearby energies (see Fig. 4.7).

The values for the shortest lifetimes are of the order of a picosecond, much shorter than all previous measurements of inter-Landau level relaxation in other heterostructures. This difference is attributed to the importance of electron-LO phonon emission, which is the origin of the oscillations in lifetime. Extrapolating the data of Maran *et al.* [4] to our higher density of $6 \times 10^{11} \text{ cm}^{-2}$ gives an electron-electron scattering lifetime of ~ 10 ps. It is therefore likely that relaxation at non-MPR conditions occurs mostly via this longer-lifetime mechanism. In this system, then, application of a magnetic field allows for tuning between two different regimes: energy relaxation via LO-phonon emission at the MPR condition, and electron-electron scattering at other fields.

It is known that *inter-subband* relaxation in quantum wells is strongly dependent on the subband separation, and that once this exceeds the LO-phonon energy, lifetimes of order picoseconds or less have been observed by interband optical methods [7,8]. Theoretical models of 2D intersubband relaxation have shown enhanced cooling at the equivalent of the MPR condition [20], where the subband separation energy equals the LO-phonon energy. This mechanism has been proposed to give rise to an electrophonon effect in calculations of carrier scattering rates using the momentum conservation approximation [21,22]. Pevzner *et al.* [23] predict a similar phenomenon in 1D systems as well. Experimentally, Shank *et al.* found cooling lifetimes $\tau < 1$ ps for excited energy states in GaAs/AlGaAs multi-quantum wells (MQWs) using time-resolved absorption, when direct excitation was made above the LO phonon energy with excited carrier densities similar to those here [8]. Experimental and theoretical studies of LO-phonon–assisted cooling rates in III-V bulk materials likewise find lifetimes between 0.1 and 0.7 ps depending on carrier concentration [6,10].

Warmenbol *et al.* [24] calculate the energy relaxation rates of hot electrons in applied magnetic fields in GaAs/AlGaAs heterojunctions, but for lower carrier densities ($3.4 \times 10^{11} \text{ cm}^{-2}$), finding relaxation rates which correspond to lifetimes of tens of picoseconds. Their ladder is non-terminated, so that thermal distribution promotes electrons to high energies. Nonetheless, they predict oscillations in the relaxation rate, which result in a lifetime peak-to-valley ratio of 4-5, consistent with our observations. In practice a detailed comparison with theory is also likely to require a treatment of the energy input mechanism. There are likely to be significant differences between the present case where carriers flow upwards in energy before relaxing via phonon emission, and conventional hot electron MPR experiments in which carriers are injected at high energies and cascade downwards. In addition, the complicated scattering and relaxation process at non-MPR conditions will need to be considered.

4.6 Conclusion

The experiment presented in this chapter differs markedly from all previous 2DEG CR saturation studies, performed in GaAs/AlGaAs systems. Previous studies relied on the polaron effect to truncate the ladder of available Landau states, hence saturation was possible only for energies below the LO-phonons, and used carrier densities less than $4 \times 10^{11} \text{ cm}^{-2}$. The InAs/GaSb system, with its large band nonparabolicity, saturates even when high carrier densities suppress the polaron effect. Application of a magnetic field then allows for tuning

between regimes of electron-electron scattering and energy relaxation via LO-phonon emission.

4.7 References

- [1] E. Gornik, T. Y. Chang, T. J. Bridges, V. T. Nguyen, J. D. McGee, and W. Müller, Phys. Rev. Lett. **40** (1978) 1151.
- [2] G. R. Allan, A. Black, C. R. Pidgeon, E. Gornik, W. Seidenbusch, and P. Colter, Phys. Rev. **B 31** (1985) 3560.
- [3] M. Helm, E. Gornik, A. Black, G. R. Allan, C. R. Pidgeon, K. Mitchell, and G. Weimann, Physica **134B** (1985) 323.
- [4] I. Maran, W. Seidenbusch, E. Gornik, G. Weimann, and M. Shayegan, Semicond. Sci. Technol. **9** (1994) 700.
- [5] W. Heiss, P. Auer, E. Gornik, C. R. Pidgeon, C. J. G. M. Langerak, B. N. Murdin, G. Weimann, and M. Heiblum, Appl. Phys. Lett. **67** (1995) 1110.
- [6] R. F. Leheny, J. Shah, R. L. Fork, C. V. Shank, and A. Migus, Solid State Comm. **31** (1979) 809.
- [7] J. F. Ryan, R. A. Taylor, A. J. Turberfield, A. Maciel, J. M. Worlock, A. C. Gossard, and W. Wiegmann, Phys. Rev. Lett. **53** (1984) 1841.
- [8] C. V. Shank, R. L. Fork, R. Yen, J. Shah, B. I. Greene, A. C. Gossard, and C. Weisbuch, Solid State. Comm. **47** (1985) 981.
- [9] M. C. Tatham, J. F. Ryan, and C. T. Foxon, Phys. Rev. Lett **63** (1989) 1637.
- [10] U. Hohenester, P. Supancic, P. Kocevar, X. Q. Zhou, W. Kütt, and H. Kurz, Phys. Rev. **B 47** (1993) 13233.
- [11] R. J. Nicholas, Prog. Quantum Electr. **10** (1985) 1.
- [12] R. J. Nicholas, in *Landau Level Spectroscopy*, edited by G. Landwehr and E. I. Rashba (Elsevier, Amsterdam, 1991), p. 777.
- [13] D. J. Barnes, R. J. Nicholas, F. M. Peeters, X.-G. Wu, J. T. Devreese, J. Singleton, C. J. G. M. Langerak, J. J. Harris, and C. T. Foxon, Phys. Rev. Lett. **66** (1991) 794.
- [14] M. Inoue, H. Hida, M. Inayama, Y. Inuishi, K. Nanbu, and S. Hiyamizu, Physica **B 117** (1983) 720.
- [15] D. R. Leadley, M. A. Brummell, R. J. Nicholas, J. J. Harris, and C. T. Foxon, Solid State Elect. **31** (1988) 781.

- [16] P. Hawker, A. J. Kent, L. J. Challis, M. Henini, and O. H. Hughes, *J. Phys. Cond. Matt.* **1** (1989) 1153.
- [17] D. Oepts, A. F. G. van der Meer, and P. W. van Amersfoort, *Infrared Phys. Technol.* **36** (1995) 297.
- [18] D. J. Barnes, R. J. Nicholas, R. J. Warburton, N. J. Mason, P. J. Walker, and N. Miura, *Phys. Rev. B* **49** (1994) 10474.
- [19] T. A. Kennedy, R. J. Wagner, B. D. McCombe, and D. C. Tsui, *Solid State. Comm.* **18** (1976) 275.
- [20] S.-C. Lee, I. Galbraith, and C. R. Pidgeon, *Phys. Rev. B* **52** (1995) 1874.
- [21] J. A. Levenson, G. Dolique, J. L. Oudar, and I. Abram, *Phys. Rev. B* **41** (1990) 3688.
- [22] W. Xu, F. M. Peeters, and J. T. Devreese, *Phys. Rev. B* **48** (1993) 1562.
- [23] V. B. Pevzner, V. L. Gurevich, and G. J. Iafrate, at *Electronic Properties of 2D Systems XI*, Nottingham, 1995.
- [24] P. Warmenbol, F. M. Peeters, X. Wu, and J. T. Devreese, *Phys. Rev. B* **40** (1989) 6258.

Chapter 5

Coupled Cyclotron Resonance

In this chapter I introduce coupling into the standard cyclotron resonance experiments. There are two classes of experiments, both involving new elements along the z-axis (growth direction) of the heterostructure. In the first case, I deal with magnetic field components in the superlattice planes. In the second case, I deal with light polarized in the growth direction. Each type of coupling introduces new transitions, either due to changes in the band structure, or to changes in the transition selection rules. From these new transitions, one can extract new and useful information about the electronic structure of the system, information not obtainable with standard cyclotron resonance methods.

5.1 INTRODUCTION	92
5.2 SUBBAND-LANDAU-LEVEL-COUPLING.....	92
5.2.1 EXPERIMENTAL SETUP	92
5.2.2 THEORY	94
5.2.3 RESULTS AND DISCUSSION	98
5.3 GRATING-COUPLED CYCLOTRON RESONANCE.....	101
5.3.1 EXPERIMENTAL SETUP	101
5.3.2 THEORY	103
5.3.3 RESULTS.....	103
5.4 CONCLUSIONS.....	106
5.5 REFERENCES	107

5.1 Introduction

One of the principal features of standard cyclotron resonance (CR), as noted in the previous chapters, is the physical and theoretical simplicity of the Faraday configuration. This simplicity is due to the decoupling of the equations of motion in the x and z directions, that is, between the growth direction and the planes of the material layers. In this chapter I discuss experiments where coupling has been re-introduced between the two directions. Although this makes quantitative description of the results more difficult, it allows for the determination of a number of properties not possible in standard cyclotron resonance. Most importantly, there are several simple qualitative results that are very useful in characterizing heterostructures, and in particular coupled cyclotron resonance gives information about the superlattice subbands.

The first set of experiments, subband-Landau-level-coupling (SLLC), introduce a component of magnetic field in the superlattice layer planes. This affects the electronic structure of the superlattice, distorting the zero-field band structure as the field is increased. In this case, subband and Landau levels mix, so that transitions of an intersubband-like character are allowed at normal incidence. The second set of experiments, CR performed with a grating evaporated on the surface of the sample, introduce strong components of far-infrared radiation polarized in the growth direction. Here the band structure of the superlattice is unaltered, but new transitions are observed due to the additional polarization of light.

Given that both methods aim to elucidate subband transitions, one might expect the two to give similar experimental features. In fact, the two methods give quite different features, insofar as subband transitions are concerned. This difference is perhaps expected once the opposite nature of each technique is considered: in subband-Landau-level-coupling, one is manipulating the magnetic field while keeping the incident radiation untouched, while in grating-induced coupling, the incident radiation is manipulated while the magnetic field remains in the growth direction.

5.2 Subband-Landau-Level-Coupling

5.2.1 Experimental Setup

The setup for a SLLC experiment is basically identical to standard cyclotron resonance, with one exception: the sample is tilted with respect to the field. Since the

dielectric constant of these III-V materials is large ($\epsilon \approx 13.5$), the incident far-infrared radiation remains polarized in the plane of the superlattice layers, even for large tilting angles. The magnetic permeability is of the order of unity, hence the magnetic field inside the sample will be pointing at an angle (the tilt angle) to the growth direction. The experiment therefore takes place under the condition of normally incident radiation, but with a tilted magnetic field.

SLLC was first observed in 2D systems by Beinvogl and Koch [1], who applied tilted magnetic fields to an accumulation layer in *n*-type Si. This was followed by a detailed theoretical explanation from Ando [2], who showed how the induced coupling between subbands and Landau levels led to new transitions. Doezema *et al.* [3] studied the effect of a parallel field (a field applied parallel to the layers, not to the growth direction), finding curious oscillations in the conductance of an accumulation layer in *n*-type InAs. These oscillations were determined to be points at which hybridized subband-Landau levels crossed the Fermi level.

In general, three regimes of CR behavior are observed. For small tilt angles and/or field strengths, the magnetic field is essentially a small perturbation upon the growth direction band-edge potential, and so the subbands experience only a small diamagnetic shift with Landau levels following the “ $B \cos \phi$ ” law (described below). For large angles and strong magnetic fields, the cyclotron orbit is smaller than the layer thickness, so that bulk CR is recovered. For in-between field strengths and tilt angles, there is a hybridization of subband and Landau levels, and it is through this hybridization that new transitions are observed.

The first SLLC experiments performed on the InAs/GaSb system were performed by Maan *et al.* [4], who studied the optical response of very wide layer superlattices (1000 Å InAs, 1000 Å GaSb), essentially a multiple-heterojunction structure. They studied only electron cyclotron resonance, finding that as the tilt angle increased the effective mass increased slightly, in agreement with the results presented below. In addition, at high tilt angles (30° or more) and high photon energies they observed an additional transition at fields above the CR line (indicating a lower effective mass for the new transition). This additional resonance was most likely related to the E_0 - E_1 intersubband transition in their sample, although they do not speculate.

Bluyssen *et al.* [5] studied tilted-field CR in an *n*-type thin layer InAs/GaSb sample, finding that the resonances in their case roughly followed the $B \cos \phi$ law, thereby implying that no SLLC occurred. For their sample the InAs thickness was 65 Å, so that the subband

separation was several hundreds of meV, and therefore it is not surprising that no coupling was observed.

Further work in the GaAs/AlGaAs system [6-10] has refined the analysis used. In particular, SLLC can be used to provide an estimate of the strength of the coupling matrix elements, as well as to determine intersubband separation energies.

5.2.2 Theory

Calculations were performed in the effective mass approximation (EMA), described in Chapter 2 and used to model the samples in Chapter 3. To solve the tilted-field structure in the EMA, one begins with the tilted-field Hamiltonian [2,7]

$$H = \frac{1}{2m^*} [(p_x + B z \sin \phi)^2 + (p_y + B x \cos \phi)^2 + p_z^2] + V(z), \quad (5.1)$$

where m^* is the electron effective mass, z is the growth direction, B is the total applied magnetic field, ϕ is the tilt angle, and $V(z)$ is the superlattice band-edge potential. The total Hamiltonian is then split into separate z -dependent terms, x,y -dependent terms, and the coupling term, of the form

$$\begin{aligned} H_z &= \frac{1}{2m^*} (p_z^2 + z^2 B^2 \sin^2 \phi) + V(z), \\ H_{xy} &= \frac{1}{2m^*} (p_x^2 + p_y^2 + 2 x p_y B \cos \phi + x^2 B^2 \cos^2 \phi), \\ H_{xz} &= \frac{z p_x B \sin \phi}{m^*}. \end{aligned} \quad (5.2)$$

Although Eq. (5.2) looks rather complicated, in fact it is not terribly different from Eq. (3.2), describing standard cyclotron resonance. To solve this system, the coupling term H_{xz} is ignored to begin with, and the Hamiltonians H_z and H_{xy} are solved independently. The coupling term is then re-introduced as a perturbation, so that the final tilted field states are linear combinations of solutions to the decoupled system.

The H_z term describes an electron bound in a superlattice potential, with an additional term ($z^2 B^2$) coming from the planar-direction magnetic field, and so can be solved numerically. There are two important complications when solving H_z , however. The first

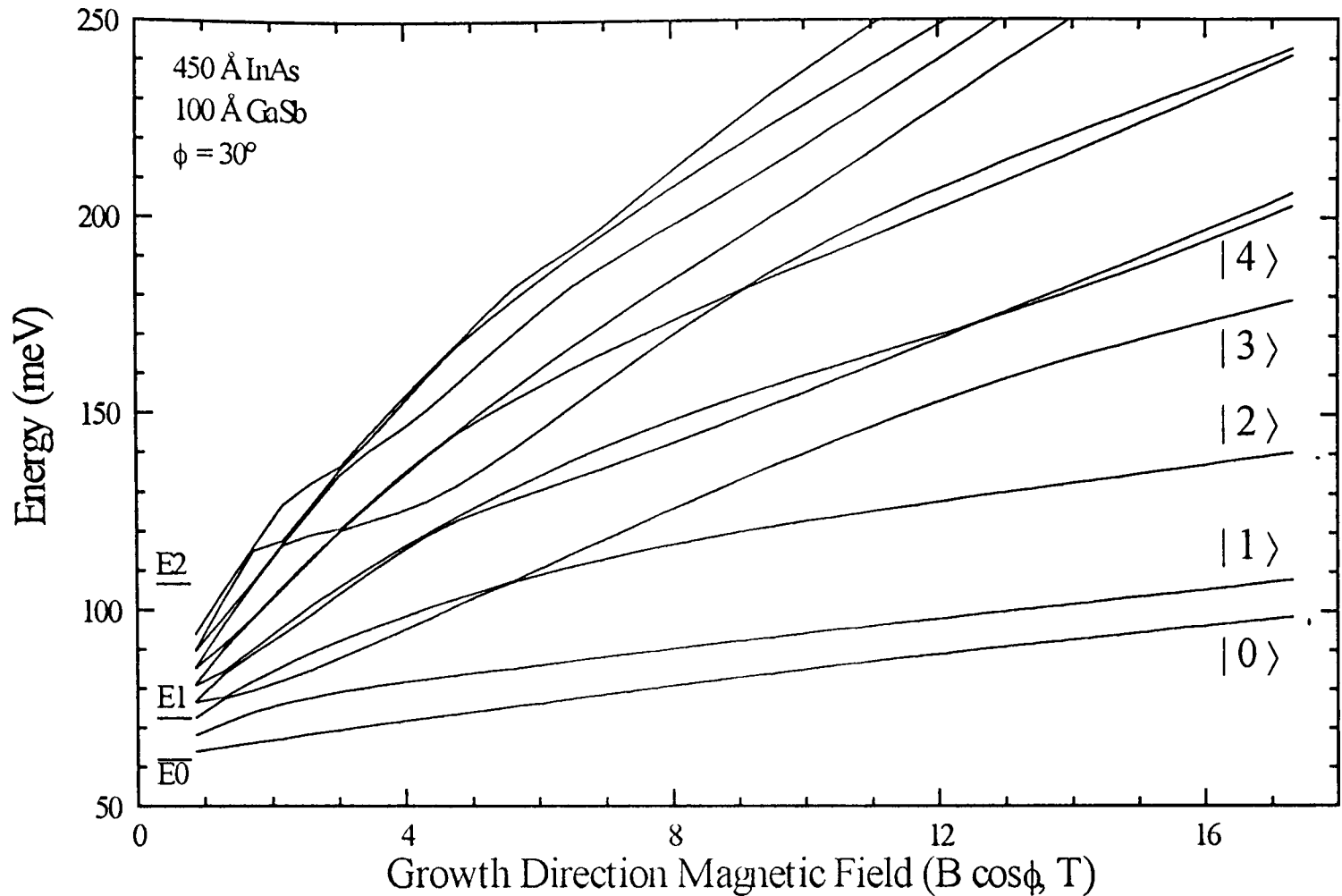


Figure 5.1: The first few hybridized energy levels of a wide-layer InAs/GaSb superlattice in a tilted field (30° to the growth direction). The zero-field subband energies are labeled on the left. The tilted field introduces strong coupling between the Landau levels of the subbands, causing anticrossings (such as the small one at $B \sim 2$ T, and the large one at $B \sim 5$ T). The hybridized state notation is labeled on the right.

point is that the superlattice condition $V(z+cl) = V(z)$ is now broken, due to the parabolic nature of the magnetic field confinement term. In practice, this is not difficult to work around, as the electrons are considered to be strongly bound in their respective InAs wells. For the EMA calculations, the wide layer widths encountered in semimetallic structures tend to result in decoupled quantum wells, rather than coupled superlattice states. Therefore, the semimetallic superlattices are modeled as a multi-quantum well structure.

The second complication in solving H_z is more subtle. With the form of H_z in Eq. (5.2), the Hamiltonian is suddenly quite sensitive to the choice of the z origin. Before, in zero-field calculations, the choice of origin was irrelevant. Now, with an explicit z^2 term, setting $z = 0$ in the middle or edge of the InAs layer will have drastic consequences on the resulting energy structure. In effect, setting the z origin amounts to determining the center of oscillation as the electron orbits in the applied magnetic field. It is known that the choice of this “center coordinate” will influence the band structure considerably [1,4].

To solve H_z , the same self-consistent EMA algorithm is employed as was used in Chapter 3, similar to the model described in ref. [15]. In addition to Coulombic band-bending, the expectation value $z_i = \langle i | z | i \rangle$ is computed for each subband i , and this z_i is then used as

the center coordinate in the next iteration. For [001] superlattices, the center coordinate is found to correspond to the center of the InAs well for all populated subbands. For [111] superlattices, the center coordinate is expected to shift somewhat from the center, due to the effects of the piezoelectric field. Here I solve only the [001] orientation. The end result of solving H_z is a series of subbands, with energies and wave functions slightly modified from their zero-field values.

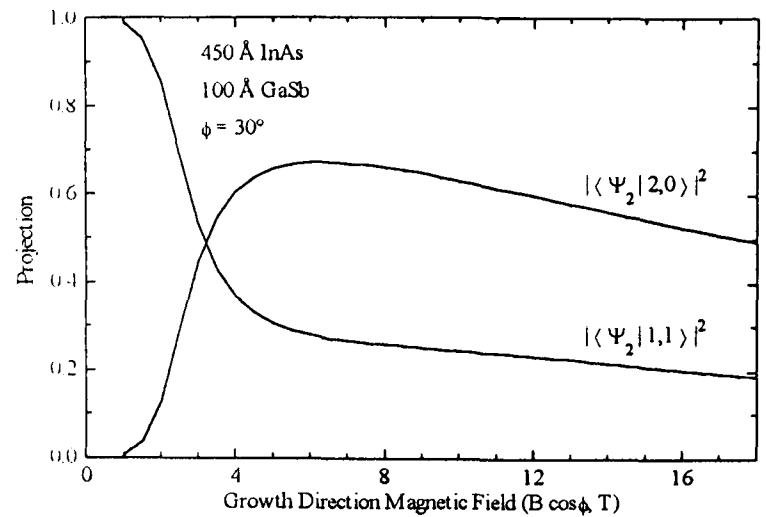


Figure 5.2: Change in character of a hybridized state as it experiences an anticrossing.

Solving H_{xy} is exactly the same as solving Eq. (3.5). Again, a canonical transformation removes the $x p_y B$ coupling term, and the result is a series of harmonic oscillator wave functions and energies, differing by a constant frequency $\omega_c = e B \cos \phi / m^*$. The form and method of solution in this case and in standard CR are identical: the only difference is that B has been replaced by $B \cos \phi$. For small fields (or small tilt angles) the magnetic field is a small perturbation on the band-edge potential, and so the resonances are expected to obey this “ $B \cos \phi$ ” law [7].

At this point in the calculation, the band structure is very similar to the standard CR structure: the electron motion is decoupled in the growth and planar directions, resulting in decoupled energy states. Each subband n will have associated with it an infinite number of Landau levels, which cross the Landau levels of other subbands.

To include the coupling term H_{xz} as a perturbation (or, equivalently, to express solutions of the total Hamiltonian as a linear combination of the decoupled H_z and H_{xy} solutions), one constructs the matrix

$$M_{nN'nN} = \langle n'N' | H | Nn \rangle, \quad (5.3)$$

where n is the subband index, and N is the Landau level index. Diagonalization of Eq. (5.3) results in the tilted-field subband energies. The eigenvector corresponding to each energy contains the coefficients of the basis $|nN\rangle$ states, and so allows for calculation of the tilted-field wave functions. For convergence, the first five subbands have been included, and the first ten or so Landau levels associated with each subband (the number Landau levels included

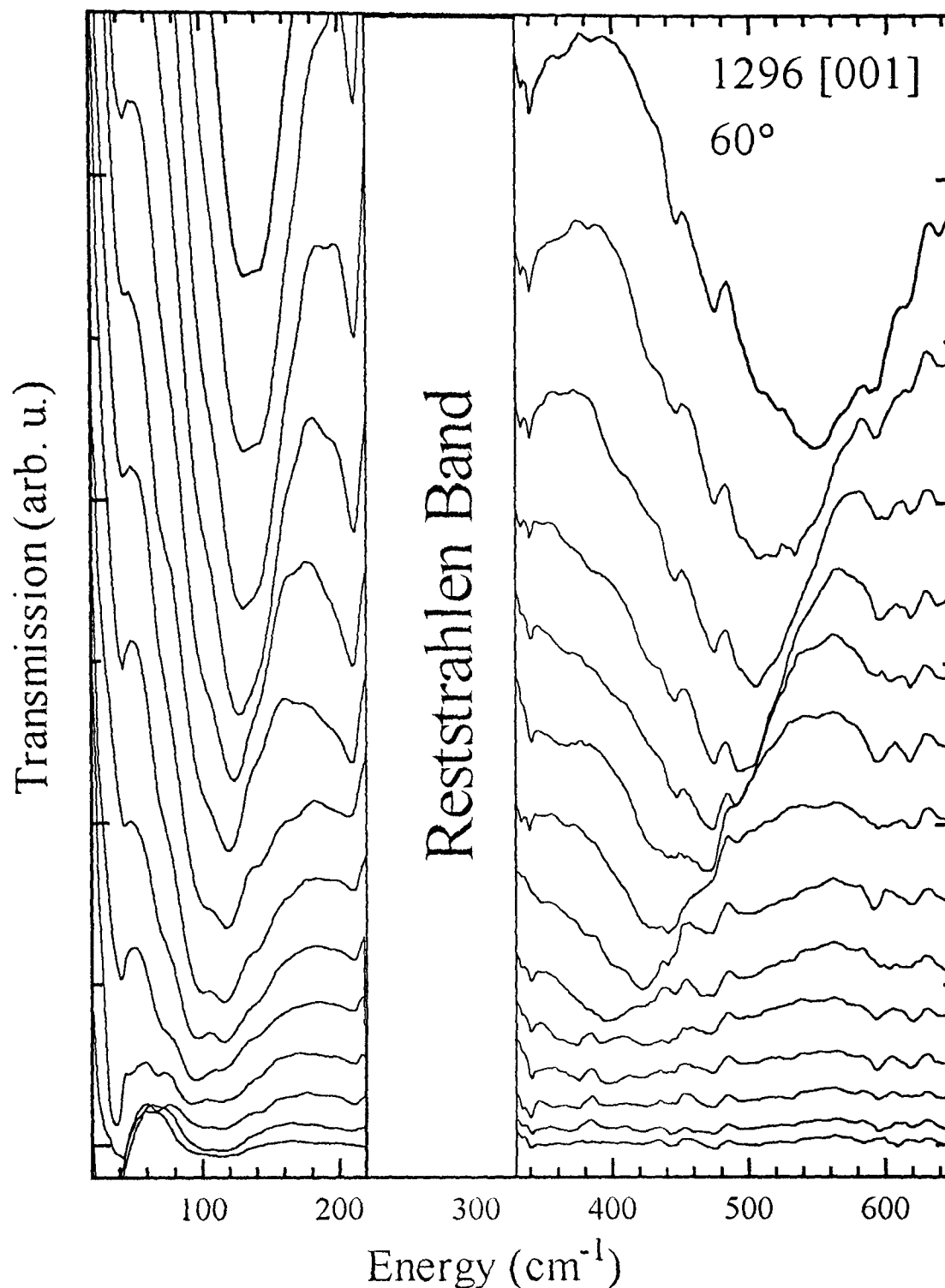


Figure 5.3: The energy spectra of sample 1296 [001] at a tilt angle of 60° . The spectra start at the top at 14 T, and decrement in 1 T steps.

depends on the strength of the field and the tilt angle, in general a small value of $B \cos \phi$ requires many Landau levels). With the energies and wave functions of the tilted field states thus established, it is straightforward to calculate the transition matrix elements between states, and so to predict transitions.

The Landau fan for one wide-layer superlattice in a magnetic field tilted at 30° is presented in Fig. 5.1. The $n = 1$ Landau level of the 0^{th} subband (state $|0,1\rangle$) anticrosses with state $|1,0\rangle$ at $B \sim 2$ T. The $|1,1\rangle$ and $|2,0\rangle$ states experience strong repulsion at $B \sim 5$ T. The anticrossings lead to a change in band character, where in this case the hybridized state $|\Psi_1\rangle$ changes from predominantly $|0,1\rangle$ to $|1,0\rangle$. The state $|\Psi_2\rangle$ likewise changes from $|1,1\rangle$ to $|2,0\rangle$ (see Fig. 5.2).

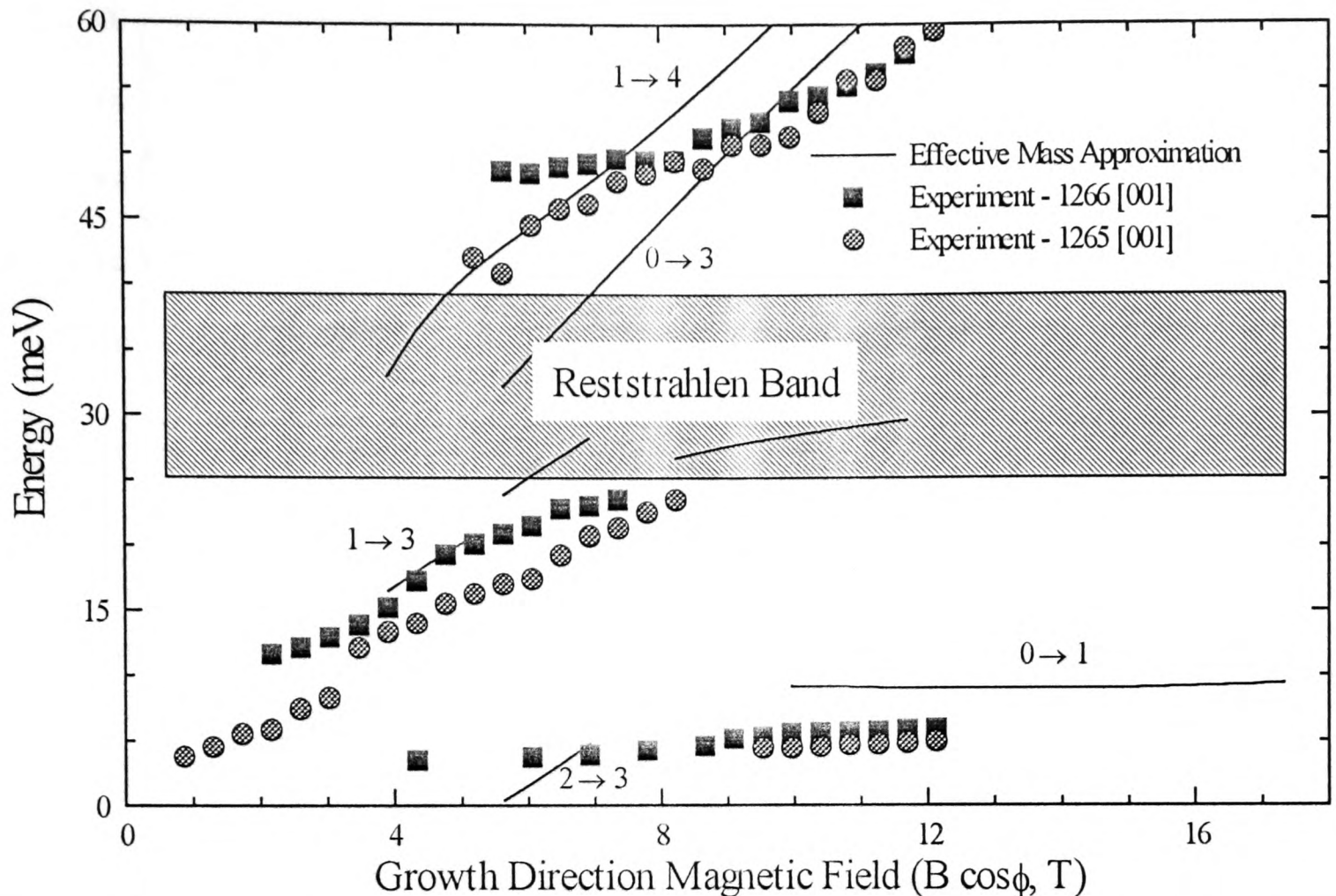


Figure 5.4: A comparison of theory and experiment at a tilt angle of 30° . The transitions are between states as labeled in Fig. 5.1.

Due to the $z p_x$ nature of the H_{xz} coupling term, states which repel the strongest are likely to have the strongest optical coupling at normal incidence, so that these anticrossings are expected to result in nonlinear transitions in field.

5.2.3 Results and Discussion

Typical experimental spectra are plotted in Fig. 5.3 for sample 1296 [001] at a tilt angle of 60° . At this tilt angle, it is clear that the $B \cos \phi$ approximation is no longer valid, as two different strong electron resonances are visible, above and below the reststrahlen.

In Fig. 5.4 the resonance energies are plotted as a function of field for samples 1266 [001] and 1265 [001] at a tilt angle of 30° . Both samples have similar growth parameters (450 Å InAs, 100 Å GaSb). The electron cyclotron resonance has been split into upper and lower branches, above and below the reststrahlen band. This indicates an E_1 - E_2 subband separation energy somewhere in the reststrahlen band, in agreement with the EMA calculations. The E_0 - E_1 transition is expected at energies around 10 meV. However this is the same energy region as the heavy hole resonances, and so we cannot assign the transitions as uniquely intersubband-like. The agreement between theory and experiment is very good, considering the approximations used.

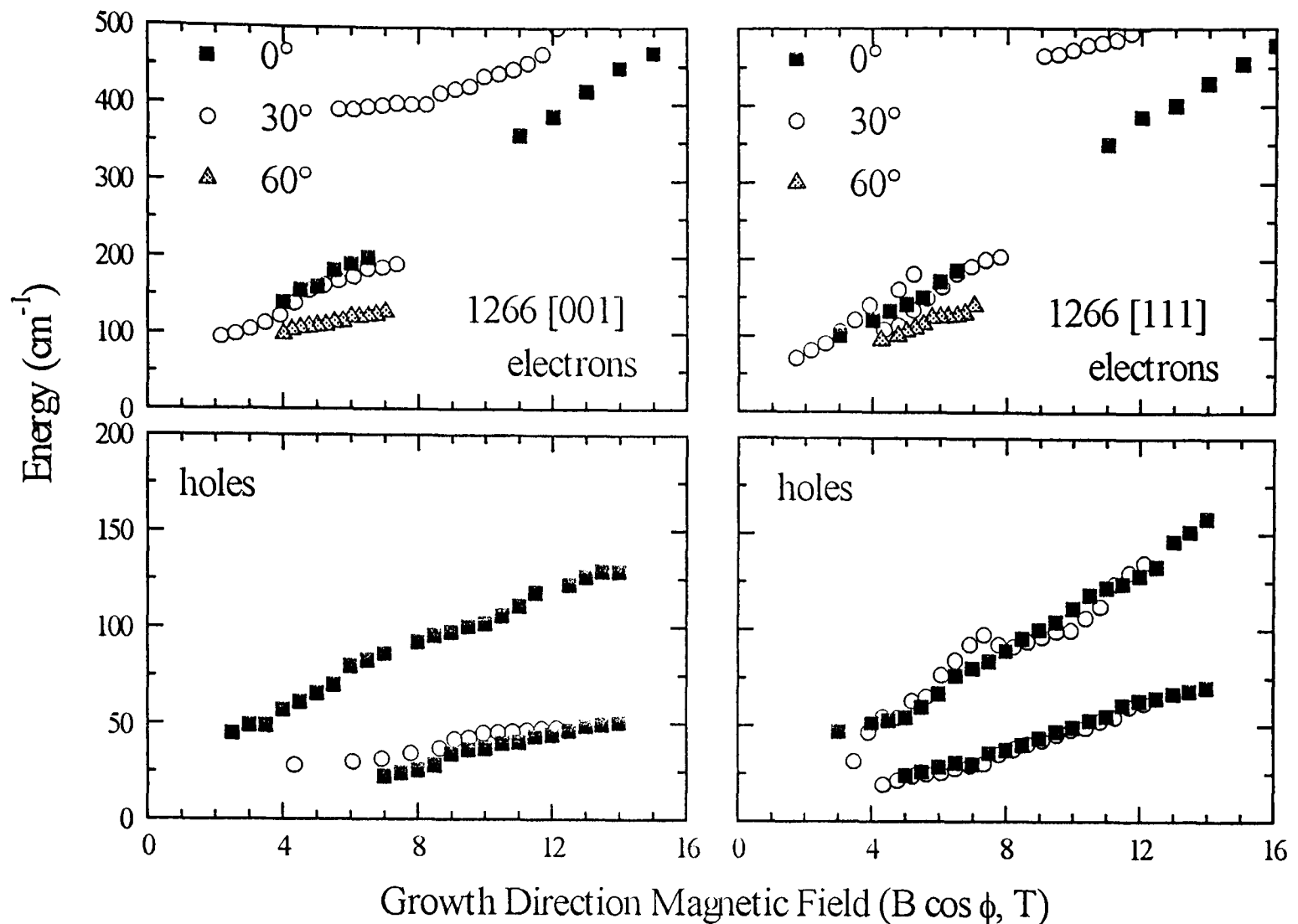


Figure 5.5: Resonance positions as a function of growth orientation and tilt angle for sample 1266 (450 Å InAs, 100 Å GaSb). For 1266 [111] at a tilt angle of 30°, there may be a splitting of the 5 T electron resonance at the condition $E_{12} = 2 \hbar \omega_c$.

Resonance positions are plotted in Fig. 5.5 for sample 1266 for the [001] and [111] growth orientations at tilt angles of 0, 30, and 60 degrees. As the tilt angle increases, the lower branch (below the subband separation energy) of the electron resonance shifts down, below the $\hbar \omega_c \cos \phi$ line. This is due to the H_{yz} coupling term, which at these tilt angles and field values strongly warps the energy bands (as in Fig. 5.1). In the same way, the upper branch shifts to higher energies, above the $\hbar \omega_c \cos \phi$ line. In contrast, the hole resonances follow the $\hbar \omega_c \cos \phi$ line for all tilt angles at which they are observed. This is possible if the hole CR energy is smaller than the hole subband separation energy for the fields investigated here, an observation with which both EMA and multi-band calculations agree.

Some samples, such as 1132 [001] and 1249 [001], exhibited no resonant coupling, with electron resonances following the $B \cos \phi$ law at all tilt angles. Resonances for sample 1132 [001] are plotted in Fig. 5.6. Much as the hole resonances, the lack of SLLC is explained if the subband separation energy is always greater than the CR energy. The EMA calculation predicts $E_1 - E_0$ separations of over 80 meV (600+ cm⁻¹) for these two samples, which is far greater than the CR energies reached at these magnetic fields [14].

Table 5.1: Observed (at 30°) and calculated z_{ii} coupling matrix elements, in Å. The EMA calculation was not performed for the [111] orientation.

Sample	Observed	Calculated
1265 [001]	74	85
1266 [001]	104	85
1266 [111]	106	--
1296 [001]	84	51
1546 [001]	93	85

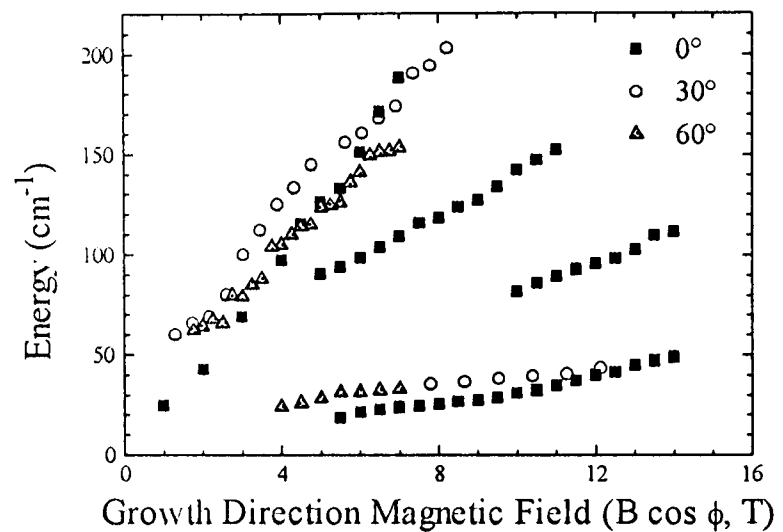


Figure 5.6: Resonance energies as a function of magnetic field and tilt angle for sample 1132 [001]. No SLLC is observed.

Rikken *et al.* [7], Wieck *et al.* [8], Summers [9] and Michels [10] used SLLC as a method of probing the electronic structure of GaAs/AlGaAs heterojunctions. In those high mobility, low carrier density systems, small tilt angles were used which allowed precise determination of subband separations, matrix elements between states, and even an estimate of the depolarization shift in intersubband transitions. In contrast, the InAs/(Ga,In)Sb superlattices used here have carrier densities greater than those achieved in GaAs/AlGaAs heterojunctions, even with the strong illumination used by Wieck [8]. The high carrier densities, and lower mobilities, require larger tilting angles for the CR splitting to be resolved. At these tilt angles the first order perturbation used here is of questionable validity, although it does appear to match observed transitions very well.

Using first order perturbation theory, the matrix element z_{ii} is given by [8]

$$z_{ii} = \langle i' | z | i \rangle = \frac{l_{\perp} \Delta E}{\sqrt{2 n E_{ii} \tan \phi}}, \quad (5.4)$$

where i is the subband index, $l_{\perp} = (\hbar / e B \cos \phi)^{1/2}$ is the magnetic length, ΔE is the energy splitting between the two branches, and E_{ii} is the subband separation energy. Eq. (5.4) is derived for coupling between the n and $n+1$ Landau levels of adjacent subbands. The observed and calculated matrix elements are presented in Table 5.1. The matrix elements are somewhat sensitive to the exact values of the field at which the splitting occurs and the subband separation energy. Given the large splittings observed at 30°, these values could only be estimated. In general, the subband separation energies for all these samples was 33-37 meV, in agreement with the EMA calculation which predicts 36-40 meV.

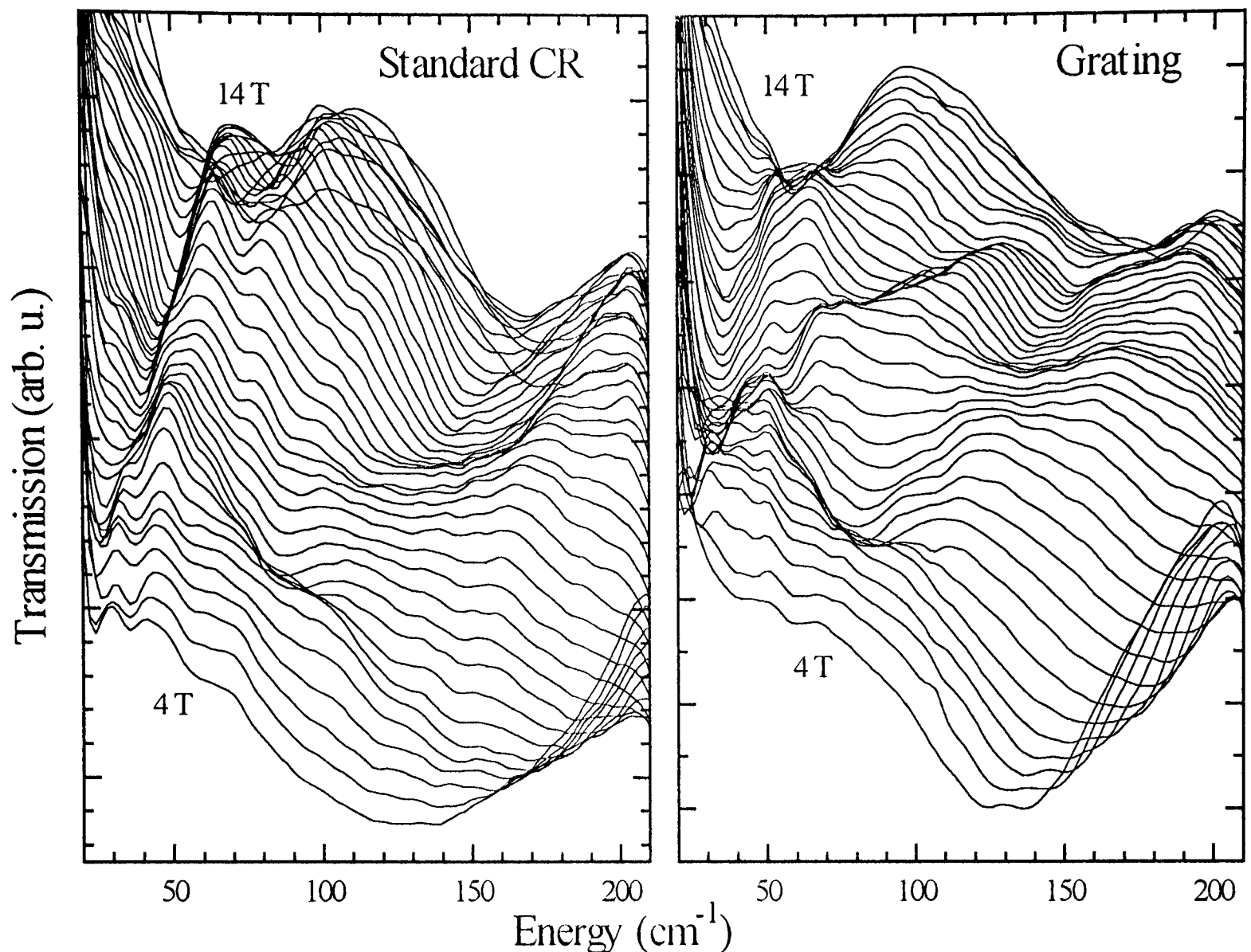


Figure 5.7: Low energy cyclotron resonance for sample 1546 [001]. The traces start at the top at 14 T, and decrement in $\frac{1}{4}$ T steps. On the left is the spectra resulting from standard CR measurements, identical to that presented in Chapter 3. On the right is the same experiment, where a metal grating has been deposited on the surface of the sample.

5.3 Grating-Coupled Cyclotron Resonance

5.3.1 Experimental Setup

For the grating-coupled CR experiments, the experimental setup is exactly as described in Chapter 3. The only difference is in the fabrication of the samples: in this case, a fine gold grating is evaporated on the surface. Four samples were grating, all wide-layer (semimetallic) 20-period superlattices. Three (1132, 1296, 1546) were grown in the [001] orientation, and one (1296) was also grown in the [111] orientation (specifically the [111]A orientation, see Chapter 3). The grating consisted of closely-spaced ($5\text{ }\mu\text{m}$ period) lines of gold, each $3\text{ }\mu\text{m}$ wide. The rapid modulation of dielectric constant at the surface of the sample leads to interesting radiation coupling effects, coupling which depends on the geometry of the grating and the wavelength of the incident radiation. For the purposes of this experiment, the gratings were optimized such that there is a strong component of incident far-infrared radiation

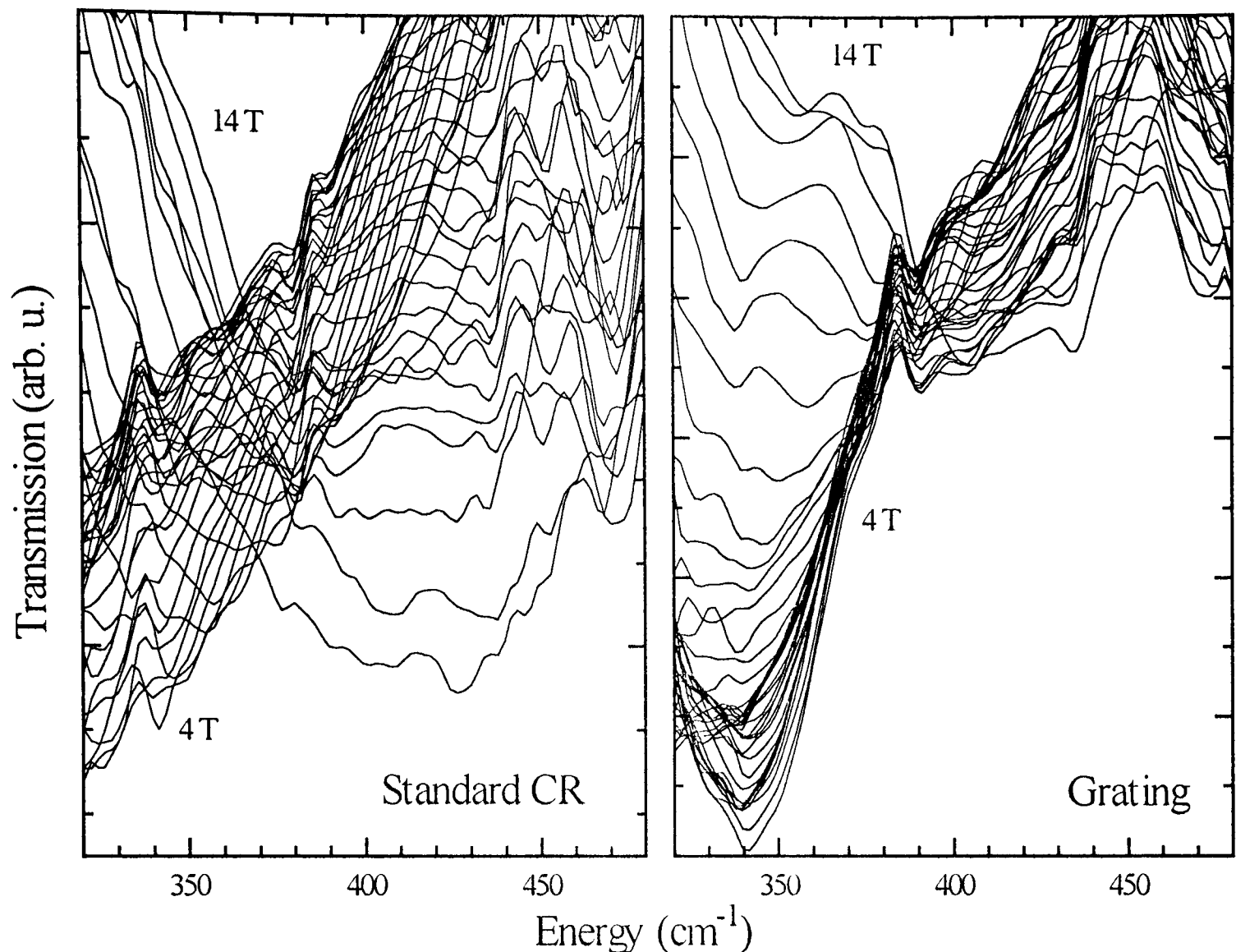


Figure 5.8: High energy spectra for 1546 [001]. The traces start at the top at 14 T, and decrement in 0.25 T steps. On the left is standard CR spectra, on the right is spectra obtained from a piece of 1546 with a metal grating deposited on the surface.

polarized in the growth direction of the superlattice, even for normally-incident light. CR experiments with grating samples therefore take place under conditions of a growth-direction magnetic field, with far-infrared radiation essentially polarized in *all* directions. New transitions are expected, owing to the new polarization of light now available, but the standard CR transitions observed in Chapter 3 should be observed as well.

Theoretical work by Nee [11] and Goossen and Lyon [12] have demonstrated the expected benefits of an applied grating. In the case of Goossen and Lyon, they found that the quantum efficiency of an intersubband detector rose from 1% to over 90% when a grating was applied. Experimental work by Li *et al.* [13] demonstrated that the efficiency of a grating depends on the ratio of the wavelength to the grating period. Extrapolating their results, we expect a coupling efficiency of ~3% for these gratings and average transition energies of 35 meV.

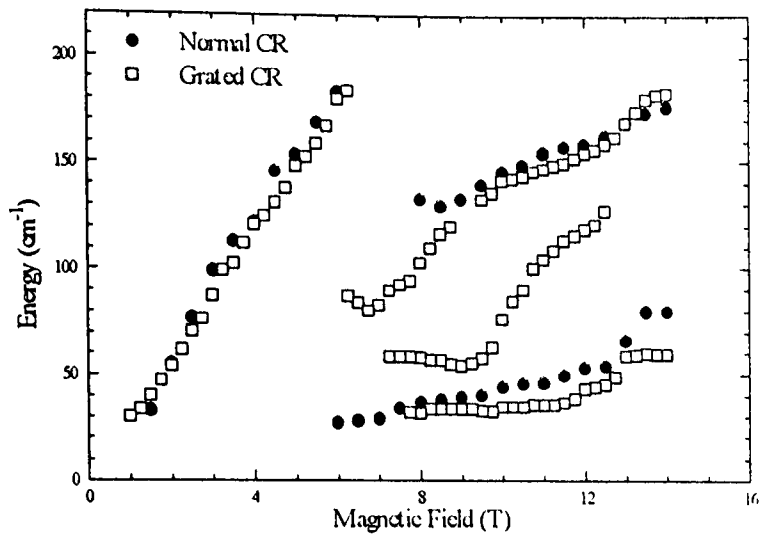


Figure 5.9: Resonance position as a function of field, for sample 1546 [001] with and without a grating.

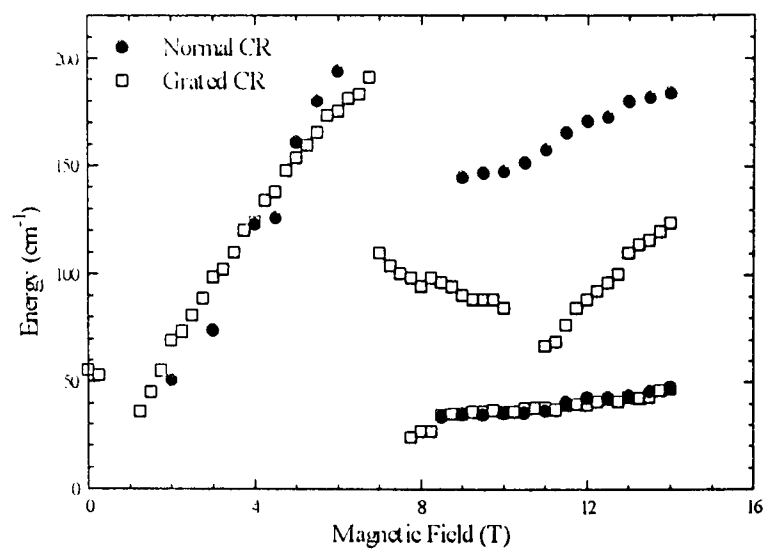


Figure 5.10: Resonance position as a function of field, for sample 1296 [001] with and without a grating.

5.3.2 Theory

Exact modeling of the effects of a grating on a sample is a complicated undertaking, particularly for 2D systems [11]. For the purposes of comparing experiment with theory, the only assumption made here about the grating is that it introduces strong components of infrared radiation polarized in the growth direction. This alters the selection rules presented in Chapter 2. In particular, Chapter 2 assumed that the incident radiation was a mixture of left- and right-circular polarizations (normally incident light). With a grating on the surface, an additional polarization vector is added, for a total polarization of $\epsilon = \epsilon_+ + \epsilon_- + \epsilon_z$. This (for a magnetic field applied in the growth direction) introduces a new term in the transition matrix element $\langle i | \epsilon \cdot p | f \rangle$, of the form

$$\sum_{m,n}^{\Gamma} \int_0^d f_{im}^* p_z f_{fn} dz \delta_{mn} \delta_{j(f,n),j(i,m)}. \quad (5.5)$$

The new allowed transitions are therefore between the same Landau levels of different subbands.

5.3.3 Results

Low energy spectra for one sample, 1546 [001], are presented in Fig. 5.7. The effect of a grating is clear: existing transitions are somewhat sharpened, and new transitions are also observed. The high energy spectra are presented in Fig. 5.8. In the high-energy region of standard CR, the electron resonance moves to lower energies as the magnetic field is

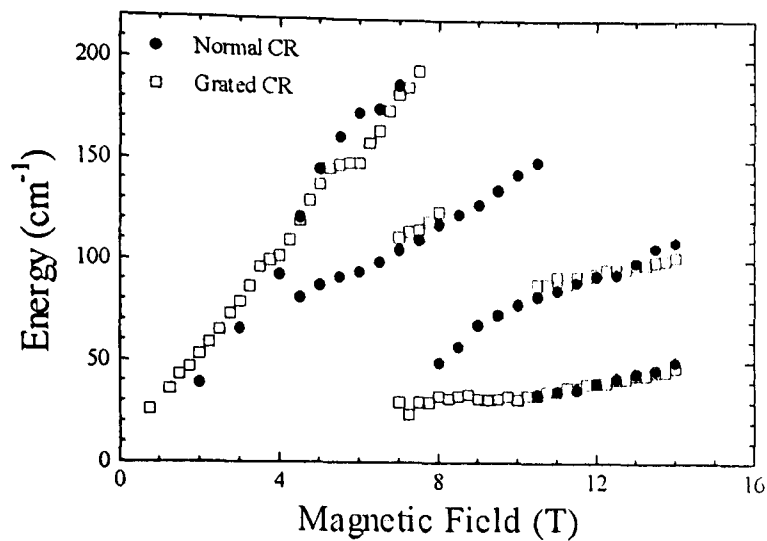


Figure 5.11: Resonance position as a function of field, for sample 1132 [001] with and without a grating.

new transitions are almost certainly due to the strong component of light polarized parallel to the layers. This new light polarization enhances intra-conduction band transitions (since conduction states are strongly *s*-type, which in a heterostructure allows absorption only for electric field components in the growth direction), therefore it is expected that the observed grating-induced transitions are related to conduction subbands.

The resonance positions are plotted as a function of magnetic field for sample 1546 [001] in Fig. 5.9. Many transitions correspond to CR observed in the sample without a grating, but new resonances are clear in the region 6-12 T, 50-150 cm⁻¹. Similar new transitions are also observed in sample 1296 [001], plotted in Fig. 5.10. Samples 1132 [001] and 1296 [111] exhibited no new low-energy transitions, although 1132 [001] did show evidence for a field-independent resonance at 48 meV (the resonances from sample 1132 [001] are plotted in Fig. 5.11).

The constant resonances at high energies (above the reststrahlen band) are assumed to be related to intersubband transitions, due to their lack of magnetic field dependence and the fact that the resonances only appear with an applied grating. Because of the even symmetry of the potential in [001] structures, it is expected that only transitions between subbands of opposite parity will be allowed. Likewise, it is assumed that observed transitions occur between the highest occupied and lowest unoccupied electron subbands. This indicates an E_1 - E_2 separation of roughly 42 meV in sample 1546 [001], an E_1 - E_2 separation of 42 meV in 1296 [001], and an E_0 - E_1 separation of 48 meV in 1132 [001]. The number of subbands populated (2 in both 1546 and 1296, and 1 in 1132) are determined from transport measurements [15], which agree with the self-consistent calculations presented in Chapter 7. Those calculations predict energy separations of 30, 45, and 82 meV for 1546, 1296, and

decreased, quickly disappearing into the reststrahlen band (220-320 cm⁻¹). With a grating, the additional polarization of light allows an intersubband transition, which persists at ~340 cm⁻¹ for all fields.

The sharpening of the transitions is most likely due to impedance matching, where the grating smoothes the transition from a region of low impedance (atmosphere or vacuum) to high impedance (the sample). The

1132 respectively, similar to EMA results [14]. Likewise, SLLC results (presented above) and further grating analysis (presented below) indicate subband separations of 30-35 meV for 1546 and 1296. These constant high-energy resonances are therefore substantially different from the observed subband separation energies. For 1546 and 1296, the new resonances lie above the subband separation, while for 1132 the resonances are somewhat

below the expected separation. Although depolarization and exciton-like shifts are expected to shift the intersubband resonances somewhat [16], the observed transitions cannot be explained by those shifts, which are on the order of $\sim 10\%$.

The new low-energy resonances (between the heavy and light heavy holes) show a striking field-dependence. At high fields they are “CR-like,” that is, they increase in energy as the field increases. At low fields, they are “anti-CR-like,” where their energy decreases as the field is increased.

In Fig. 5.12 a simple parabolic model is proposed to explain the observed new low energy transitions. It is proposed that the Landau levels of adjacent subbands couple, in a similar manner to the tilted field case. However, the magnetic field is strictly in the growth direction, therefore any coupling must be a consequence of band mixing. Depending on mixing and population effects, transitions from the $n+1$ Landau level of the ground subband and the n Landau level of the first excited subband will be allowed in a range of magnetic fields near their crossing point. As in the tilted field case, these transitions are allowed due to the mixing of character of the bands in the region of the crossing. Here the grating-induced polarization component of light in the growth direction will allow intersubband transitions, and it is this intersubband character of the bands which allows the normally forbidden n to $n+1$ transition between Landau levels of adjacent subbands.

There are four qualitative aspects to Fig. 5.12. First, the CR-like transitions are expected to be parallel to the normal electron resonances, as is observed. Second, the anti-CR-like resonances will occur at lower field values, such that CR-like and anti-CR-like resonances never occur at the same field, which again is observed. The third point is that at a given magnetic field, the energy difference between the normal electron resonances and the

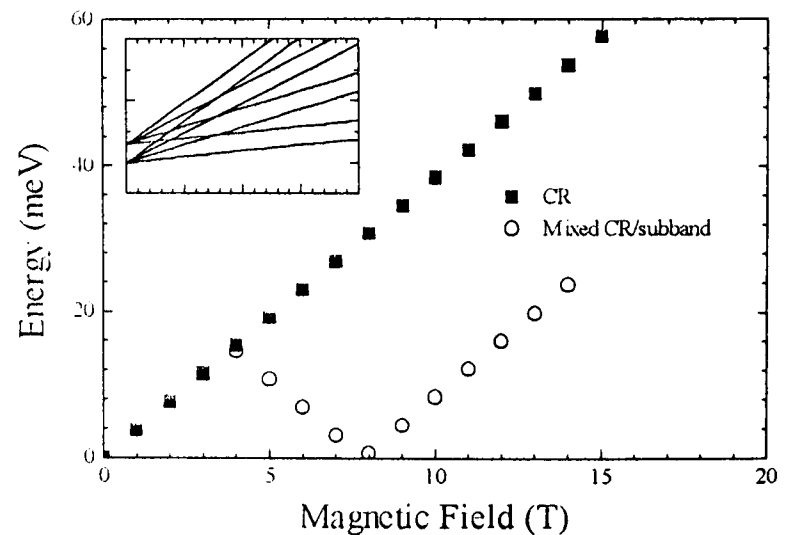


Figure 5.12: A simple parabolic model to explain observed “anti-CR” transitions. The Landau levels used to generate these transitions are inset.

Table 5.2: Subband separation energies and coupling determined from coupled CR experiments. E_{ij} is the intersubband transition energy, ΔE is the coupling energy. All densities (n and p) are given in 10^{11} cm^{-2} , all energies are in meV.

Sample	n	p	Calculated E_{ij}	SLLC E_{ij}	Grating E_{ij}	SLLC $\Delta E/E_{ij}$	Grating $\Delta E/E_{ij}$
1132 [001]	7.0	3.1	82	--	--	--	--
1296 [001]	7.5	3.4	45	35	32	54 %	25 %
1296 [111]	15.1	6.2	42	--	--	--	--
1546 [001]	7.2	4.6	30	29	28	48 %	24 %

new CR-like resonances is exactly the intersubband spacing. Therefore, the CR-like resonances allow a direct determination of the intersubband energies.

The fourth point is that in Fig. 5.12, the new transitions actually reach zero energy at some point (~ 8 T in this case), a “turning point” where the transitions switch from CR- to anti-CR character. This turning point occurs at zero energy in this simple model only because the lack of coupling allows the Landau levels to be degenerate at their crossing point. If coupling is included, then the levels will anticross, leading to a turning point at non-zero energies. Just as in the tilted-field case, the energy of the turning point provides a measure of the intersubband coupling matrix element.

The intersubband energies derived in this way for sample 1546 [001] and 1296 [001] are 28 and 32 meV respectively, in good agreement with the tilted-field results (see Table 5.2). These results are expected to be more accurate, since in the tilted field case the intersubband energy is assumed to lie somewhere between two groups of resonances, whereas in the grating case the intersubband energy is measured directly as a difference between observed resonances. In the tilted field case (at 30°) the coupling energy ΔE is 50% or more of the subband separation, whereas in this case the coupling energy (energy of the turning point) is 25% or less of the subband separation. Therefore it is concluded that the band-mixing-induced coupling is less than half the strength of the coupling induced by a 30° tilt angle.

5.4 Conclusions

In this chapter, coupling is re-introduced into the standard CR experiment, leading to several qualitative changes in the observed resonances. When the sample is tilted with respect to the magnetic field, the electron CR “splits” into two branches, one branch below the subband separation energy, and one branch above. From the energy position the intersubband energies can be deduced, and from the energy between the two branches the coupling matrix element can be estimated.

With a grating applied to the surface of a sample, incident radiation is strongly polarized in the growth direction, allowing new transitions to be observed. This leads to a new line of low energy CR-like and anti-CR-like resonances. From the position of the CR-like resonances relative to the normal electron CR, the intersubband separation is determined. From the energy of the turning point of the new resonances, the strength of the coupling can be compared to tilted-field experiments.

Although the nature of coupling makes exact comparisons between theory and experiment difficult, the simple qualitative results are a powerful tool in exploring the electronic structure of these thick-layer InAs/(Ga,In)Sb superlattices.

5.5 References

- [1] W. Beinvogl and J. F. Koch, Phys. Rev. Lett. **40** (1978) 1736.
- [2] T. Ando, Phys. Rev. **B 19** (1979) 2106.
- [3] R. E. Doezema, M. Nealon, and S. Whitmore, Phys. Rev. Lett. **45** (1980) 1593.
- [4] J. C. Maan, Ch. Uihlein, L. L. Chang, L. Esaki, Solid State Comm. **44** (1982) 653.
- [5] H. J. A. Bluyssen, J. C. Mann, P. Wyder, L. L. Chang, and L. Esaki, Phys. Rev. **B 25** (1982) 5364.
- [6] Z. Schlesinger, J. C. M. Hwang, and S. J. Allen, Jr., Phys. Rev. Lett. **50** (1983) 2098.
- [7] G. L. J. A. Rikken, H. Sigg, C. J. G. M. Langerak, H. W. Myron, J. A. A. J. Perenboom, G. Weimann, Phys. Rev. **B 34** (1986) 5590.
- [8] A. D. Wieck, F. Thiele, U. Merkt, K. Ploog, G. Weimann, and W. Schlapp, Phys. Rev. **B 39** (1989) 3785.
- [9] G. M. Summers, *D.Phil Thesis*, Clarendon, Oxford, 1993.
- [10] J. G. Michels, *D.Phil Thesis*, Clarendon, Oxford, 1994.
- [11] T. W. Nee, Phys. Rev. **B 29** (1984) 3225.
- [12] K. W. Goossen and S. A. Lyon, Appl. Phys. Lett. **47** (1985) 1257.
- [13] W. J. Li, B. D. McCombe, F. A. Chambers, G. P. Devane, J. Ralston, and G. Wicks, Surf. Sci. **228** (1990) 164.
- [14] M. Lakrimi, T. A. Vaughan, R. J. Nicholas, D. M. Symons, N. J. Mason, and P. J. Walker, Solid State Elect. **37** (1994) 1227.
- [15] D. Symons, *D.Phil Thesis*, Clarendon, Oxford, 1994.
- [16] F. Szmulowicz, M. O. Manasreh, C. E. Stutz, and T. Vaughan, Phys. Rev. **B 50** (1994) 11618.

Chapter 6

Semiconducting Superlattices

In this chapter, thin-layer (semiconducting) InAs/GaSb superlattices are investigated. Instead of direct optical transmission, the photoconductivity of the samples is measured as a function of the energy of incident light. Several samples are studied, demonstrating the dependence of the superlattice band gap with layer thickness. Application of magnetic field leads to a better estimate of the band gap, a measure of the quality of the superlattice structure, and to transitions between farther bands. Finally, a high-quality superlattice is gated for vertical transport, measurements confirming the suitability of InAs/GaSb superlattices for far-infrared applications.

6.1 INTRODUCTION	109
6.1.1 OVERVIEW	109
6.1.2 WHY INAS/GASB?.....	110
6.1.2.1 Device Requirements	110
6.1.2.2 Mercury Cadmium Telluride	111
6.1.2.3 Gallium Arsenide	112
6.2 LATERAL PHOTOCONDUCTIVITY	112
6.2.1 EXPERIMENT	112
6.2.2 BAND GAP VARIATION WITH LAYER THICKNESS	113
6.2.3 INTERBAND MAGNETOOPTICS	115
6.2.3.1 Experimental Results	115
6.2.3.2 Fitting with a Decoupled Model.....	116
6.2.3.3 Fitting with a $k \cdot p$ Model.....	117
6.2.3.4 Excitons.....	119
6.2.4 CONCLUSIONS FROM LATERAL PHOTOCONDUCTIVITY	121
6.3 VERTICAL PHOTOCONDUCTIVITY.....	122
6.3.1 EXPERIMENT	122
6.3.2 RESULTS AND DISCUSSION	124
6.4 CONCLUSIONS.....	125
6.5 REFERENCES.....	125

6.1 Introduction

6.1.1 Overview

As mentioned in Chapter 1, the crossed-gap nature of the InAs/GaSb system has as a useful consequence the fact that the band gap can be varied through a large range of positive and negative values. The previous three experimental chapters all dealt with negative band gap structures, that is, structures with layer widths wide enough to allow charge transfer from the GaSb hole levels to the InAs conduction levels. Those chapters, dealing exclusively with intraband transitions, constitute useful investigations of the electronic properties of the system.

In this chapter, the experiments concern thin-layer superlattices, where a positive band gap still exists. Although intersubband transition engineering may render semimetallic superlattices useful in the far-infrared (see Chapter 7), the most promising immediate application of the InAs/GaSb system is this thin-layer, semiconducting system. In particular, InAs/GaSb superlattices are expected to be as good or better than bulk HgCdTe in detecting far-infrared radiation [1-4]. It is in these experiments on semiconducting samples, therefore, that we come closest to real device performance and evaluation, and study interband transitions for the first time.

Although the InAs/GaSb system has been studied since the late 1970's [5], it was not until the late 1980's that the far-infrared device potential of the strained-layer InAs/(Ga,In)Sb superlattice system was realized [1]. Early measurements relied on transport and cyclotron resonance of predominantly n-type semiconducting samples to deduce carrier densities and effective masses, which in turn provided estimates of the band gap [6,7]. Voisin *et al.* [8] observed luminescence in very thin-layer InAs/GaSb superlattices ($d \sim 70 \text{ \AA}$), with band gaps around 250 meV, with temperatures between 4 and 300 K. Miles and Chow *et al.* [9,10] reported 4 K optical far-infrared response of InAs/(Ga,In)Sb superlattices in 1990, with photoconductivity experiments on superlattices grown with band gaps between 70 and 350 meV. These band gaps are only slightly larger than those presented here, but their layers were somewhat thinner, as they incorporated 25% indium into the barriers. Campbell *et al.* [11] grew an 83-period thin-layer InAs/(Ga,In)Sb superlattice with 35% indium, observing a 100 meV absorption cut-off at 300 K, after the substrate had been thinned to 70 μm . Omaggio *et al.* [12] observed interband response in magnetic field at 4 K, extrapolating to ~ 100 meV band gaps and carrier effective masses similar to those observed here. In general,

however, the Omaggio data did not include as many higher-order transitions as are observed here, most likely due to the greater layer-thickness-fluctuation sensitivity of thin-layer superlattices. Katz *et al.* [13] observed strong absorption at 100 meV in a p-type InAs/GaSb superlattice at 77 K, where coupling with the conduction band was used to provide light heavy-hole masses, and so increase the absorption strength. Most recently, Hasenberg *et al.* [14] have fabricated a 3.5 μm InAs/(Ga,In)Sb superlattice diode laser, observing lasing action at temperatures up to 160 K.

Youngdale *et al.* [15] find recombination lifetimes in optimized InAs/(Ga,In)Sb superlattices to be an order of magnitude or more longer than in bulk HgCdTe at a temperature of 77 K, but much shorter at 300 K. Their work indicates that optimal far-infrared devices should be designed with thin (Ga,In)Sb layers and should operate at liquid nitrogen temperatures. Further theoretical work has confirmed that the InAs/(Ga,In)Sb system has the longest Auger lifetimes and strongest optical matrix elements when the barrier layers are made as thin as possible [16-18].

The strengths of the InAs/GaSb system relative to other materials are discussed below. The great weakness of the system is well-known to all researchers: the spatial separation of carriers leads to vanishing optical matrix elements as the layer widths increase. Another problem, common to all heterostructures, is the effect of layer width fluctuations on the sharpness of the band gap response. The experiments in this chapter have three purposes: to investigate the electronic structure of semimetallic InAs/GaSb superlattices (particularly band gaps and effective masses), to study the effect of thick layers on the absorption, and to determine the sensitivity of the band gap response to layer fluctuations.

6.1.2 Why InAs/GaSb?

This chapter is optimistic in its assessment of the promise of InAs/GaSb heterostructures as far-infrared devices. Although shortcomings of the system are discussed here and in Chapter 7, the outlook is positive. There are many far-infrared materials already in use on the market, so why is so much attention focused on this system in particular?

6.1.2.1 Device Requirements

Any comparison of material systems will be made in terms of device applications [19]. A successful material system must meet the following requirements:

Reasonable wavelength range of operation: To be of practical use, the system must be useful over a sizable range of far-infrared wavelengths, from a few microns out to 20+ μm .

Absorption/Emission Physics: The system must absorb strongly for normally incident light, and (particularly for emitters), should have long non-radiative recombination lifetimes. The bulk material $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$ (discussed below) is the current standard far-infrared material, and so is the “benchmark” with which to compare absorption and lifetimes.

Mature growth technology: The growth of the material system should be well-understood, lead to consistent structure across a substrate wafer, and should be reasonably inexpensive (or, at worst, reasonably expensive).

Device Applications: The material system should be easily integrable, possibly with some electronics on-chip. The device should perform well at high temperatures (80-200 K).

With these requirements in mind, the InAs/GaSb system is compared with current and prospective far-infrared material systems.

6.1.2.2 Mercury Cadmium Telluride

Mercury cadmium telluride ($\text{Hg}_x\text{Cd}_{1-x}\text{Te}$, or MCT for short) is the current industry standard far-infrared material. It is a bulk system, where the alloy composition is varied to adjust the band gap (the band gap decreases as the mercury content increases). As a bulk material, it exhibits fairly strong absorption in the far-infrared at any incidence.

MCT has one problem inherent to the physics of the system: as all small band gap systems, it suffers from very light effective masses. These light masses lead to large tunneling currents at finite temperatures, basically noise. The carriers in the InAs/GaSb system, however, are on the order of 5-8 times heavier than their MCT counterparts, with a corresponding reduction in tunneling current.

The biggest problem with MCT, however, is the growth technology. Growth of II-VI materials is in general a difficult and expensive process, but the problem is magnified in MCT by the sensitivity of the band gap to alloy concentrations, particularly in the far-infrared region ($\lambda \geq 8 \mu\text{m}$). Slight variations in mercury concentration across the sample lead to regions of

bulk with different effective band gaps. In addition, as an alloyed system, MCT is subject to ordering, again with deleterious consequences for band gaps, consistency, and reproducibility across the wafer.

6.1.2.3 Gallium Arsenide

Gallium Arsenide is often claimed to be the successor to silicon in a variety of applications. Certainly GaAs has already made headway into the semiconductor market, by way of HEMTs. GaAs' future as a far-infrared material remains in doubt, however.

GaAs enjoys a well-understood, inexpensive growth technology. Even InAs/GaSb devices will most likely be grown on GaAs substrates, due to their high quality and (most importantly) low cost. The main problem with GaAs is that as a Type-I system whose fundamental band-gap is in the near-infrared, any far-infrared absorption *must* be accomplished via intersubband transitions. However, as shown in Chapter 2, intersubband transitions are not allowed at normal incidence, except when mixing with far bands is taken into account. Even with far-band mixing, normal absorption within the conduction band (the easiest structure to engineer) is exceedingly weak.

This problem is avoided in two ways: a grating (or more complicated structure) can be defined on the surface of the structure, coupling light in the growth direction, or one can work with p-type samples. In either case, however, intersubband transitions are usually far weaker than interband transitions (simply because momentum matrix elements between Bloch basis states are much larger than between subband envelope functions). The fact that the InAs/GaSb system allows normally incident interband absorption at far-infrared wavelengths is its chief advantage over GaAs. Even for very long wavelengths ($\lambda \geq 20 \mu\text{m}$), where interband absorption in InAs/GaSb is negligible due to carrier separation, intersubband absorption may be strong at normal incidence, as conduction and valence states mix heavily with each other.

6.2 Lateral Photoconductivity

6.2.1 Experiment

All of the samples in this study were grown on [001] GaAs substrates at atmospheric pressure in the Clarendon MOVPE reactor, following growth of a thick ($\sim 1 \mu\text{m}$) GaSb buffer layer. InAs thicknesses ranged from 40 to 75 Å, with GaSb to InAs thickness ratios close to 1:1. Details for each sample are presented in Table 6.1. The samples were not intentionally

Table 6.1: Growth, characterization, measurement, and theoretical data at 2K for the six samples studied. N is the number of periods grown, E_G is the band gap.

Sample No.	N	Interface type	SL Period (Å)	Observed E_G (meV)	k·p fit InAs/GaSb (Å)
1625	20	GaAs	91	221	41/50
1694	20	Alternating	87	138	60/27
1697	100	Alternating	148	125	55/93
1698	100	Alternating	146	61	75/71
2037	71	InSb	113	~ 90-140	63/50
2072	80	GaAs	75	~ 150-180	57/18

doped. Growth was terminated by a 2000 Å GaSb capping layer to insulate the superlattice from surface effects, a larger capping layer than usually applied to semimetallic systems. Within the superlattice itself, interfaces were biased as either ‘GaAs’, ‘InSb’, or were alternated. The period of each superlattice as given in Table 6.1 was determined from Raman measurements of folded longitudinal acoustic phonons, and measurements taken by transmission electron microscopy (TEM).

All samples show low-temperature freeze-out, indicating semiconducting behavior (positive band gap). The GaSb buffer layer freezes out at temperatures below 40 K, so that far-infrared photo-conduction in the samples is dominated by superlattice states. This freeze-out of carriers leads to high resistivities, on the order of $10^5 \Omega/\square$, which in turn provide for strong photoconductivity response.

The lateral photoconductivity measurements were performed at 2 K under a constant magnetic field, using a Fourier transform infrared spectrometer and a superconducting magnet. The samples were mounted in the Faraday configuration. The experimental set-up is almost identical to the standard CR set-up as described in Chapter 3, except that we make ohmic contacts to the superlattice layers. This is the origin of the term “lateral” photoconductivity: excited carriers will flow laterally, through the planes of the superlattice layers. Even poor-quality samples (not presented here) gave a broad bandgap response, while high-quality samples gave clear interband response, with a well-defined Landau structure.

6.2.2 Band Gap Variation with Layer Thickness

An examination of the zero-field spectra provides a basis for comparison of band gap response of different superlattices. In addition, most device applications will require operation without an applied magnetic field. The zero-field spectra are therefore an indication of device performance, although none of these superlattices have been optimized for either absorption or

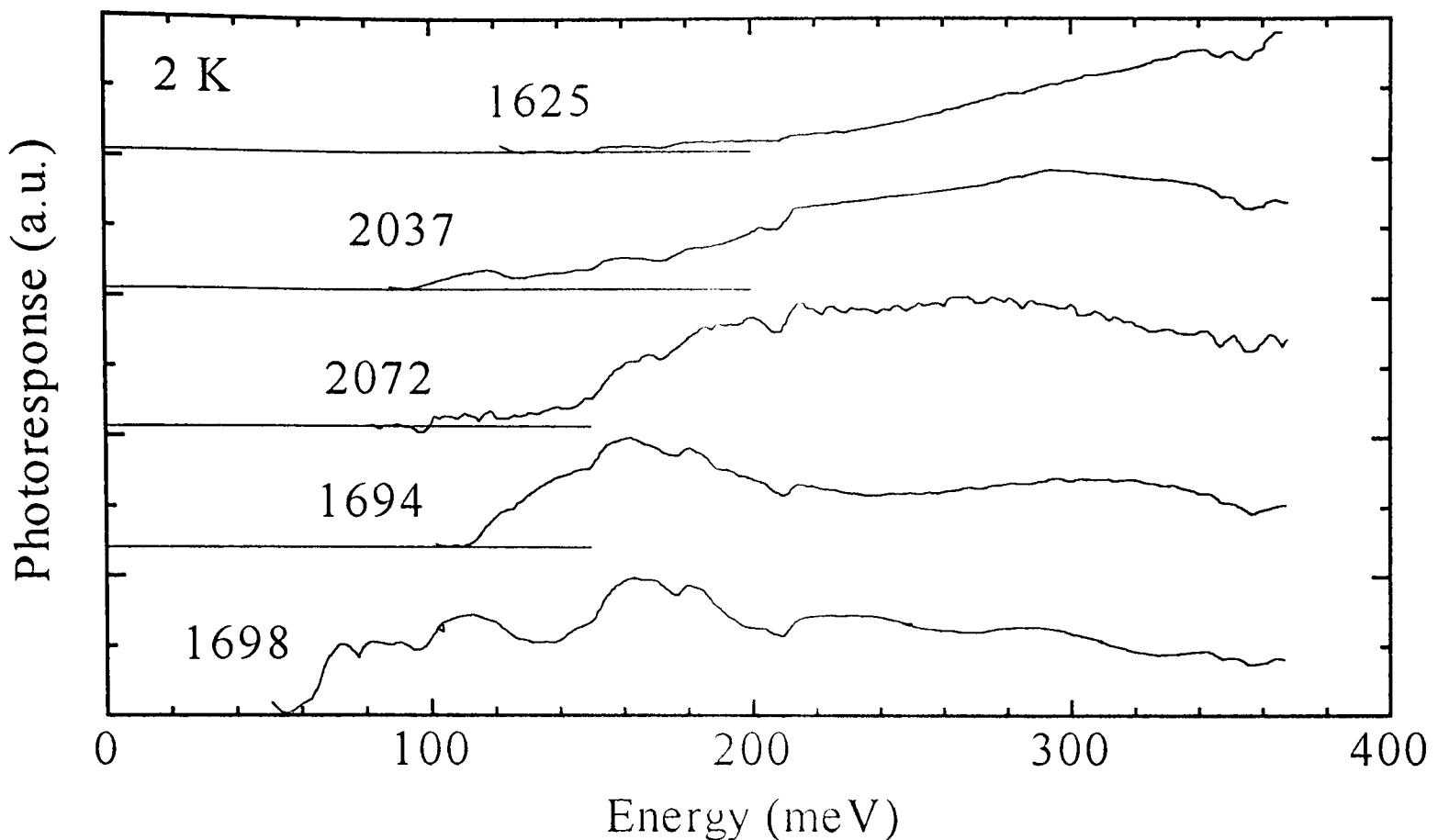


Figure 6.1: Zero-field photoresponse of several thin-layer superlattices, ratioed against the measured spectrum of the KBr window.

emission. The spectra are presented in Fig. 6.1. The observed band gaps range from around $5\ \mu\text{m}$ (sample 1625) to $20\ \mu\text{m}$ (sample 1698).

The detailed theory of zero-field absorption in thin-layer superlattices is given in Chapter 7. In summary, very strong response is expected for the thinnest superlattices, where the envelope function overlap is greatest. The wider superlattices suffer from a separation of envelope functions, leading to minuscule absorption at wavelengths much longer than $20\ \mu\text{m}$. The absorption coefficient is expected to climb sharply as the superlattice period is decreased. Surprisingly, almost the exact opposite behavior is exhibited in Fig. 6.1, where the thinnest superlattices (samples 1625, 2037) have a very broad, weak response, while the thicker superlattices (samples 1694 and especially 1698) have sharper band-edges and excellent photoresponse.

Explanation of the experimental data must therefore rely on parameters not taken into account by the theoretical model. One obvious difference between samples is simply the number of periods grown. The weak response of the thick layer superlattices may be compensated by the growth of 100 periods, whereas thinner superlattices consisted of only 20 periods. Also, the effects of fluctuations in layer thicknesses are greatest in thin samples, where even a monolayer fluctuation can correspond to 5-10% of the superlattice period. The band gaps of thin-layer superlattices are therefore much more sensitive to layer thickness

fluctuations than thick-layer superlattices. So fluctuations will lead to different layers, or even different areas of the same layer, to experience different effective band gaps. The total effect of fluctuations is then a smeared band gap response.

Further explanation of the various responses in Fig. 6.1 lies in the TEM studies. Samples 1698, 1697, and 1694 all showed very clean, regular superlattice structure. The thinner superlattices had large layer fluctuations, with step-bunching and dislocations degrading the structure. The high quality of the 1690 series has been attributed to the ease of growing thicker layers, and to different growth parameters such as temperature, gas flows, *etc.*

The important feature of Fig. 6.1 is the variation of band gap with layer thickness. Although growth irregularities may smear the response in some cases, it is obvious that as the superlattice period (and in particular, the InAs thickness) is increased, the band gap shifts to lower energies. Such behavior has of course been long predicted by theory, but quantitative experimental confirmation is crucial for devices. The weak response of some superlattices in Fig. 6.1 should not dishearten those interested in InAs/GaSb far-infrared devices, as growth improvements and tricks presented in Chapter 7 could sharpen response considerably. The absolute magnitude of the response can always be improved, either by clever structure engineering or simply by growing more superlattice layers.

6.2.3 Interband Magnetooptics

6.2.3.1 Experimental Results

To enhance the interband transition, a magnetic field was applied. All samples exhibited a strong band-edge $n = 0$ Landau transition, in some cases followed by a series of higher-order transitions. Results for one sample are shown in Fig. 6.2, with the magnetic field value given on the right hand side of each spectrum. Sample 1698 displayed the most Landau levels; on other samples, only a handful of higher transitions could be resolved. Following the selection rules for the Faraday configuration (see Chapter 2), the strongest and lowest-energy peaks are expected to correspond to $\Delta\sigma = \pm 1$, $\Delta n = \Delta\nu = 0$ (σ , n and ν are the spin, Landau and subband indices, respectively). Almost all resonances correspond to heavy-hole valence to conduction band transitions, although in some samples evidence is found for transitions between light-hole and conduction bands. However, no spin-splitting of the transitions is seen. This is not surprising, as the theory predicts splittings (at most 10 meV) which are smaller than the width of the observed transitions.

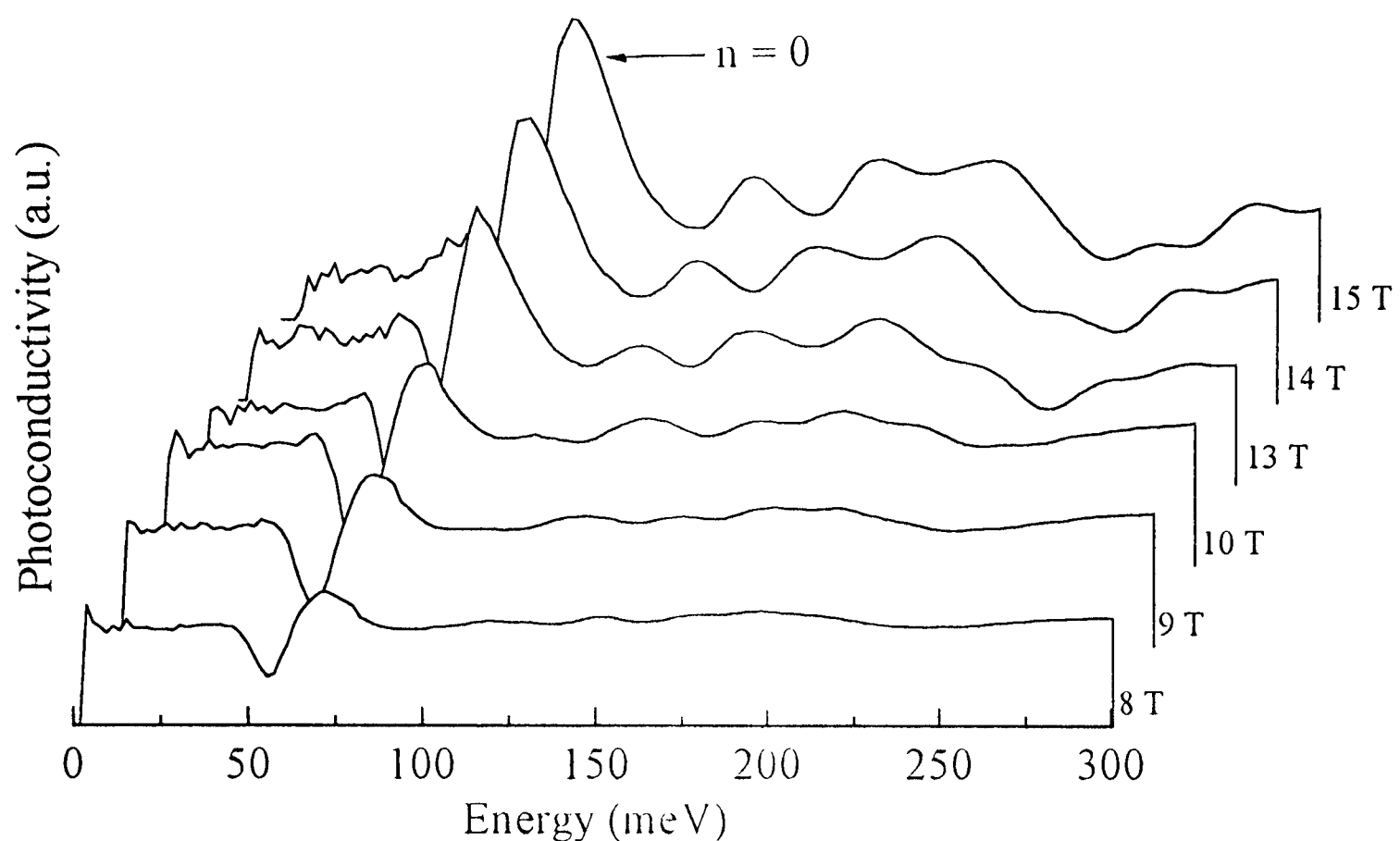


Figure 6.2: Photoconductivity spectra of sample 1698 taken at fixed field (labeled), ratioed against the zero-field response, at 2K.

6.2.3.2 Fitting with a Decoupled Model

The energies of the resonances are plotted as a function of magnetic field. The observed transitions are fitted with a simple decoupled model to determine the carrier effective masses and zero-field band gap. In the decoupled model, the transition energy for a given Landau index n is simply

$$\omega_n = E_G + \left(\frac{1}{m_e^*(E, E_G')} + \frac{1}{m_{hh}^*(E, E_G')} \right) (n + \frac{1}{2}) B, \quad (6.6)$$

where the fitting parameters are the superlattice band gap E_G , the electron and heavy-hole band-edge effective masses m_e^* and m_{hh}^* , respectively, and an effective band gap E_G' which defines the nonparabolicity.

An example of the fitted resonances is provided in Figure 6.3. The band gap and effective masses extracted in this manner are listed in Table 6.2 for this and two additional samples. The effective band gap E_G' was typically on the order of the InAs band gap

Table 6.2: Fitted superlattice parameters.

Sample No.	Fitted		
	Band Gap E_G (meV)	Fitted m_e^*	Fitted m_{hh}^*
1694	138	0.038	0.25
1697	125	0.036	0.25
1698	61	0.035	0.25

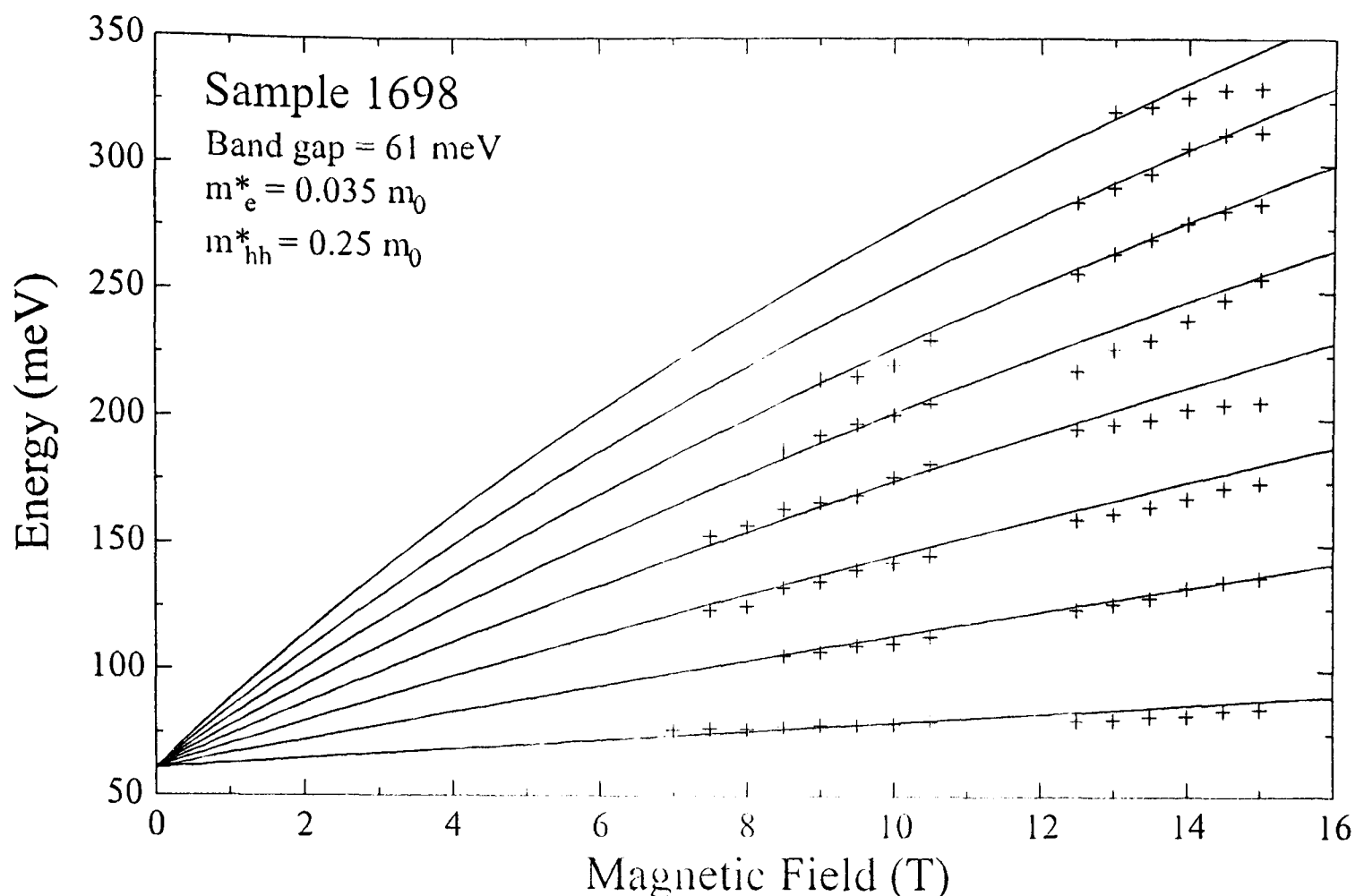


Figure 6.3: Landau transitions for sample 1698 plotted against field, fitted by transition curves from the decoupled model.

(~400 meV), to reproduce observed non-parabolicity. The observed electron effective masses (typically $m_e^* = 0.036 m_0$) are heavier than both the band-edge mass ($0.023 m_0$) and the effective mass seen in most semimetallic structures ($\sim 0.033 m_0$, see Chapter 3), indicating that the electron confinement energy is far above the InAs band-edge, as predicted by theory. The hole effective masses m_{hh}^* definitely correspond to heavy holes, with observed masses of $0.25 m_0$. As the confinement energy of the conduction band increases (InAs width decreases), the electron effective mass is found to increase as well, as expected for non-parabolic bands. The heavy hole masses were found to remain approximately constant for the GaSb widths studied, although the decoupled model is not especially sensitive to the hole masses alone.

6.2.3.3 Fitting with a $k \cdot p$ Model

This decoupled model is a useful tool for rough determination of band gaps and effective masses, but was a poor fit for some experimental data. In particular, the “best-fit” parameters for sample 1694 left several transitions unaccounted for (Fig. 6.4). For particular GaSb widths, there is likely to be considerable interaction between light- and heavy-hole Landau levels in the valence band which affect the interband Landau transitions. In addition,

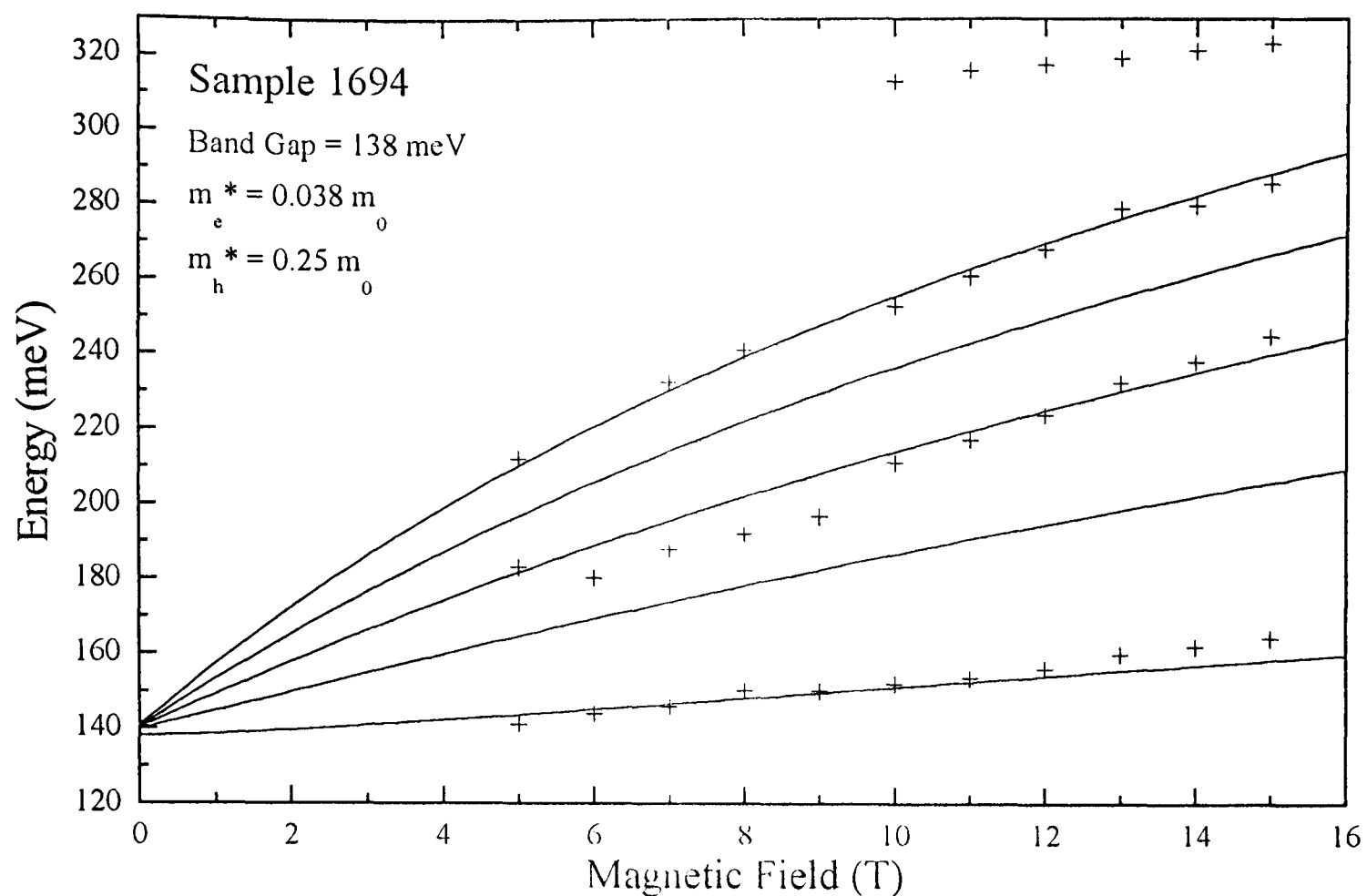


Figure 6.4: The “best fit” of the decoupled model for sample 1694. The fit predicts many absorption lines not observed in experiment. A slight exciton shift of 4 meV has been added to the $n = 0$ transition.

the bulk model cannot account for possible light-hole to conduction transitions (or transitions between higher-order subbands) without including many more fitting parameters.

To accurately model the conduction and valence band mixing, an 8-band transfer-matrix EFA calculation (essentially the Ram-Mohan model) was performed, as was outlined in Chapter 2. For each superlattice the total period thickness given in Table 6.1 was kept constant, and the ratio of the layer widths was adjusted to best match the Landau transitions. The final layer widths, listed in Table 6.1, are consistent with TEM measurements. The band overlap (defined as the energy difference between the GaSb valence band-edge and the InAs conduction band-edge) varies as a function of interface type. ‘GaAs’-like interfaces have an overlap of 140 meV, while the overlap is 100 meV for ‘InSb’-like interfaces [20]. To account for the interface mixing in these samples an average overlap of 120 meV is used. Some plots of magnetic field energy band dispersion are given in Chapter 2: here the predicted transitions are of interest. The $k \cdot p$ predictions of the Landau transitions are in excellent agreement with experiment, and suggest that some light-hole to conduction transitions may be visible. Figs. 6.5 and 6.6 are the experimental and theoretical transitions for samples 1698 and 1694, respectively. This validation of the $k \cdot p$ model is important, as $k \cdot p$ -based computer modeling is used to design superlattices with stronger optical absorption in Chapter 7.

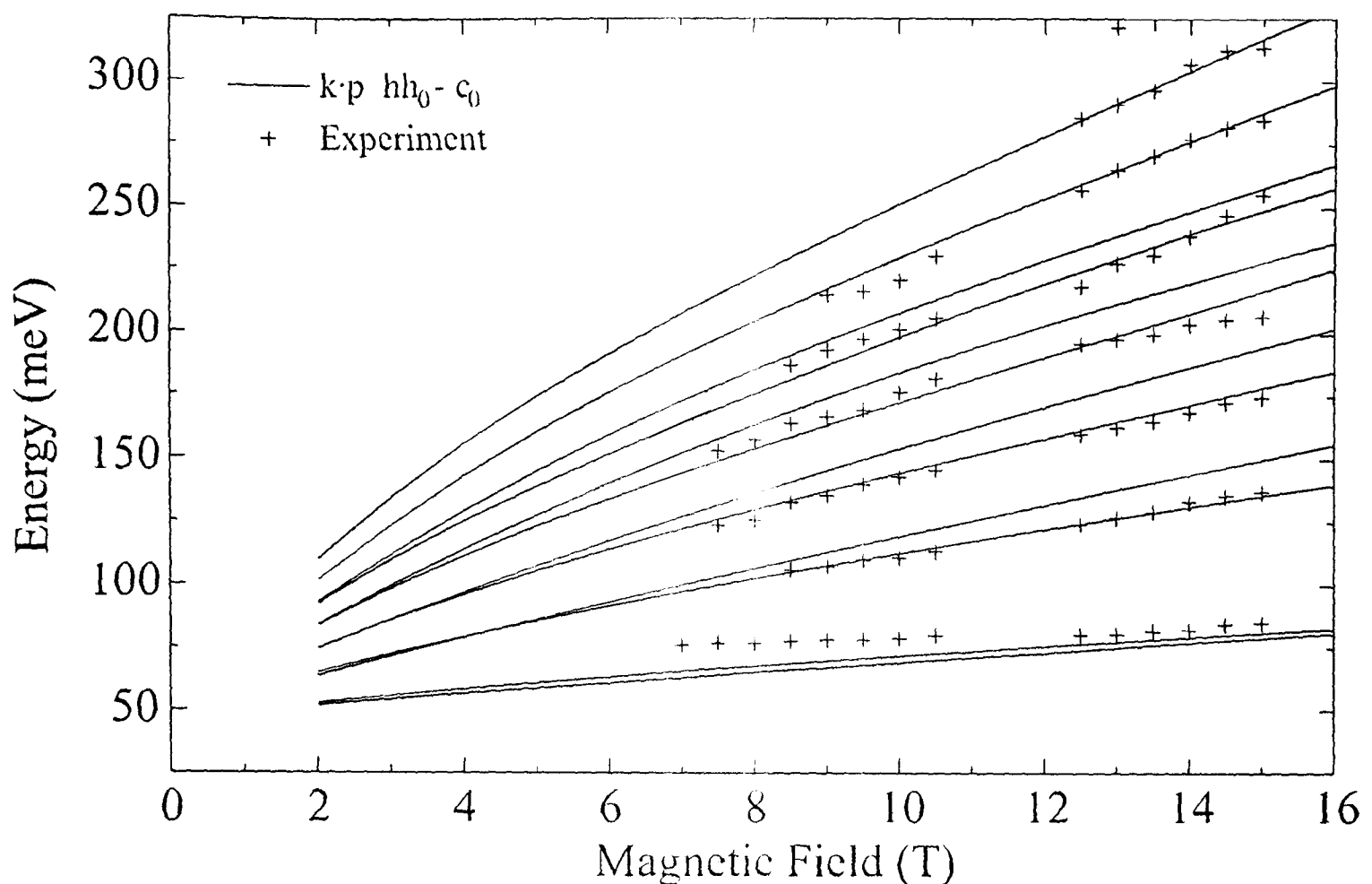


Figure 6.5: $k\cdot p$ fit for sample 1698. Theoretical spin-splitting is indicated for all but the two highest transitions.

6.2.3.4 Excitons

When fitting the photoconductivity data with the $k\cdot p$ model, accurate fitting of higher transitions in samples 1694 and 1697 was possible only if the $n=0$ transition was overestimated by ~ 8 meV (see Fig. 6.6). With sample 1698, the wealth of observed transitions led to some ambiguity as to which transitions to “best fit,” but it is possible to fit the higher transitions accurately while again over-estimating the $n=0$ transition. As in all interband transitions in magnetic field, a downward shift of the band-edge transition implies excitons.

Exciton binding energies in type-II systems are known to be small. Bastard *et al.* [21] predicted exciton binding energies of InAs/GaSb superlattices to be less than 1 meV, much smaller than in type-I systems. The smaller energies were a result of the carrier separation, so that even for very thin layers the weak wave function overlap causes the binding to decrease. The exciton binding energies were obtained by using variational wave functions, with strong decay in the barriers. We therefore expect that the greater wave function barrier penetration predicted by 8-band $k\cdot p$ methods (see Chapter 7 for examples) to increase the binding energy somewhat. Likewise, calculations by Cen *et al.* [22] in the type-II system GaAs/AlAs indicate

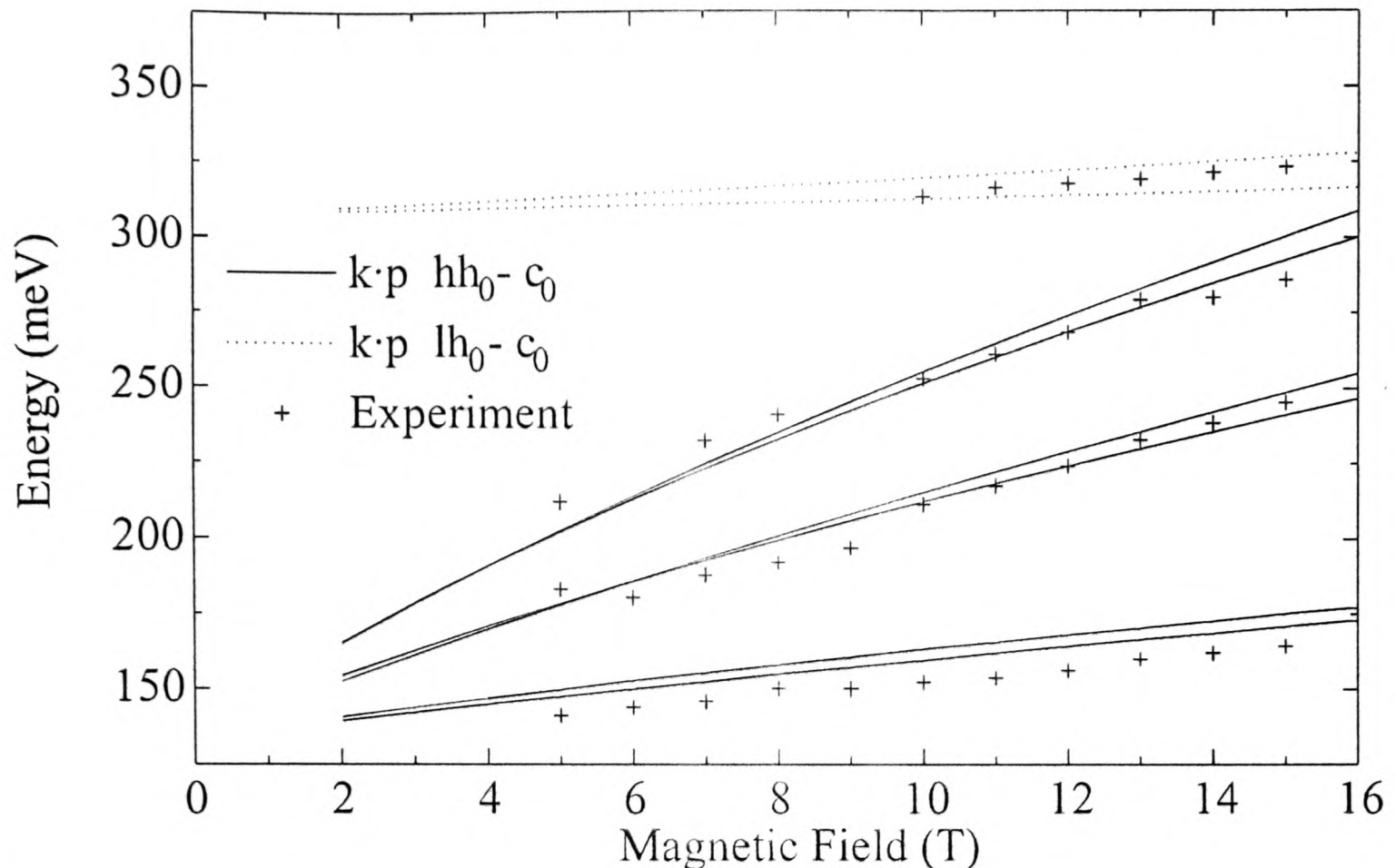


Figure 6.6: $k\cdot p$ fit for sample 1694.

that when subband mixing effects are included, the exciton binding energy can be enhanced by 50% or more over calculations which do not include coupling. These two effects, greater wave function penetration and the strong band mixing in our system, may well lead to excitons as large as several meV, possibly explaining our over-estimate of the $n = 0$ transitions in the $k\cdot p$ fitting.

Our estimate of ~ 8 meV for exciton binding energies in the InAs/GaSb system seems acceptable. Voisin *et al.* [8] observed no excitons in their photoluminescence, however the half-width at half-maximum of their 2 K spectrum was around 12 meV, and the broadening increased with temperature. Omaggio *et al.* [12] did not assume any excitons when fitting magneto-optical data similar to ours. Their fitting was performed using a two-band Kane model with three fitting parameters with at most three higher orders of transitions, where the Kane model was used to fit the observed transitions rather than for calculation of the fundamental SL electronic structure. We use an 8-band $k\cdot p$ transfer-matrix method which models the SL bound states, fitting as many as 8 or more higher-order transitions with a single fitting parameter. So it is possible that the looser fitting method used by Omaggio masked the exciton effects. In general, it may be that the exciton binding energies are so small that their effects are not appreciated, or perhaps the intrinsic nature of MOVPE-grown samples enhances the binding somewhat.

6.2.4 Conclusions from Lateral Photoconductivity

The important result of these measurements is simply that high-quality superlattices can give sharp photoresponse in the far-infrared, and the wavelength cut-off of this response is a function of the layer widths. Although very thin superlattices ($\lambda_c \leq 5 \mu\text{m}$) have ragged photoresponse, the response of 10-20 μm superlattices indicates that the InAs/GaSb has the sharpest; strongest response where MCT has its greatest weaknesses.

The zero-field results can be compared to the work on InAs/(Ga,In)Sb superlattices by Chow *et al.* [10] who measured photoconductivity in a number of similar structures. Their superlattices (all grown by MBE) gave similar response, and a similar band gap dependence on layer thickness. Our measurements were all on MOVPE-grown samples, with somewhat larger layer thicknesses. Our measured band gaps are similar to theirs, even with wider layers, most likely due to the fact that they alloyed the barrier with 25% indium in most cases. The relatively sharp response of their short-wavelength superlattices may indicate that MBE is the optimum growth technique for very thin-layer superlattices.

The magnetic field measurements are best compared to the interband magneto-optical experiments of Omaggio *et al.* [12]. Their InAs/(Ga,In)Sb superlattices exhibited band gaps of 100 meV or more, with 1-3 higher orders of observed transitions. Their extracted electron masses ($m_e^* = 0.031 m_0$) are lighter than ours, however, as they ascribe a much lighter mass to the holes ($m_h^* = 0.030 m_0$ or less). Heavy-hole in-plane masses are expected to be much lighter in thin-layer superlattices than in bulk (see Chapter 2 and ref. [1]), however we do not expect the hole masses in our system to be lighter than the electron masses, as Omaggio suggests. *k*·*p* modeling of thin layer InAs/GaSb superlattices gives hole masses no lighter than $0.1 m_0$, although the complexity of the valence band makes it difficult to provide an exact value. Likewise, the reduced masses of our transitions are over $0.03 m_0$, whereas the Omaggio reduced masses are $0.016 m_0$ or less. Clearly he has greatly reduced hole masses, while we do not. We suspect that much of the difference lies in the fact that the Omaggio samples were grown with approximately one-half the layer thickness of our samples, with 25% or more indium incorporated into the barriers. In addition, we would be surprised if our electron effective masses were much less than those given in Table 6.2, as the ground electron subband is several hundred meV above the InAs band edge.

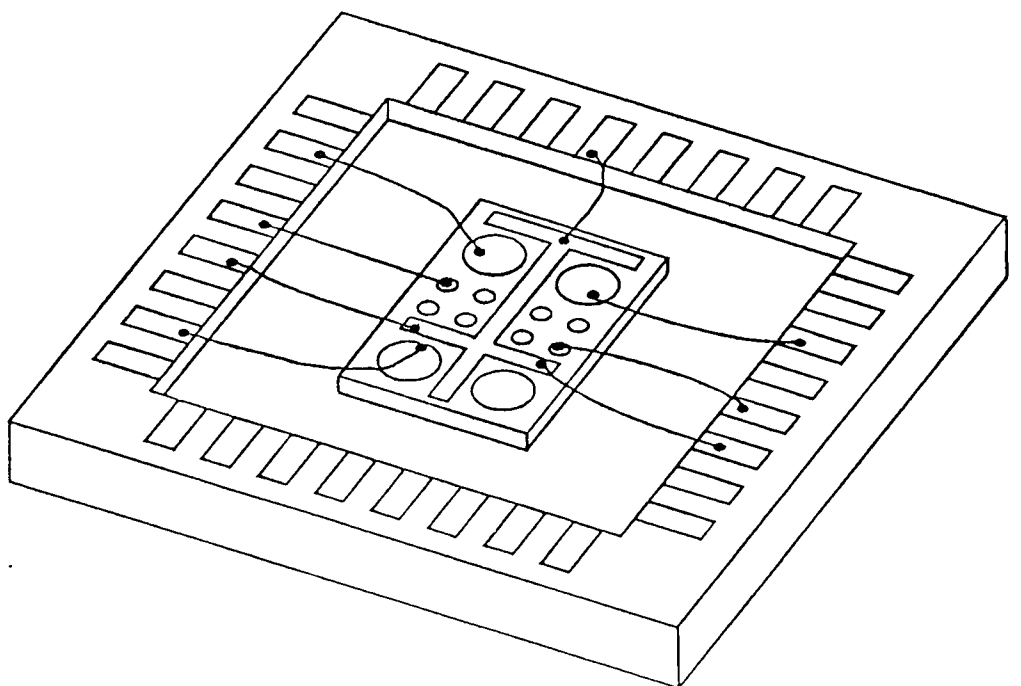
The surprising result for these experiments was the strong absorption of far-infrared superlattices, particularly samples 1694, 1697, and 1698. With no indium in the barrier,

InAs/GaSb superlattices with these band gaps are expected to exhibit weak absorption due to carrier separation. Instead, sample 1698 exhibits the longest-wavelength absorption published for InAs/(Ga,In)Sb superlattices, with a superlattice period twice as thick as any other published. The strong far-infrared response of these superlattices indicates that perhaps sharp interfaces temper the detrimental effect of carrier separation. MOVPE is therefore shown to be an excellent growth method for thick-layer InAs/GaSb systems. The inclusion of indium in the barrier is expected to improve the response of these superlattices considerably (by allowing thinner layers).

6.3 Vertical Photoconductivity

Lateral photoconductivity, as described in the section above, is an easy and useful tool to characterize semiconducting heterostructures. In real devices, however, it is impractical to measure absorption via lateral photoconductivity, simply because area of the active layer is precious, and lateral PC requires some spacing to insure electrical isolation of the contacts.

Real devices will most likely employ vertical photoconductivity, where the sample is contacted at the surface and substrate, so that current flows through the superlattice structure rather than in the plane of the layers. Much of the physics is similar: whether traveling perpendicular or parallel to the growth direction, carriers require access to unpopulated states to achieve high conduction. Thus for both lateral and vertical transport we expect good conduction when the superlattice is exposed to photons with energies greater than the band gap. The difference is simply that vertical transport requires more sophisticated sample processing.



6.3.1 Experiment

Only one sample was processed for vertical transport: the best of the lateral transport samples, 1698. Geoff Hill and

Figure 6.7: Schematic view of the vertical transport sample set-up. The sample (1698) is the small rectangle in the center, with large and small mesas (circles) evaporated on the surface. The rectangular regions on the sample are where the superlattice has been etched away, allowing contact to the substrate. The outer ceramic shell contains a number of gold contacts.

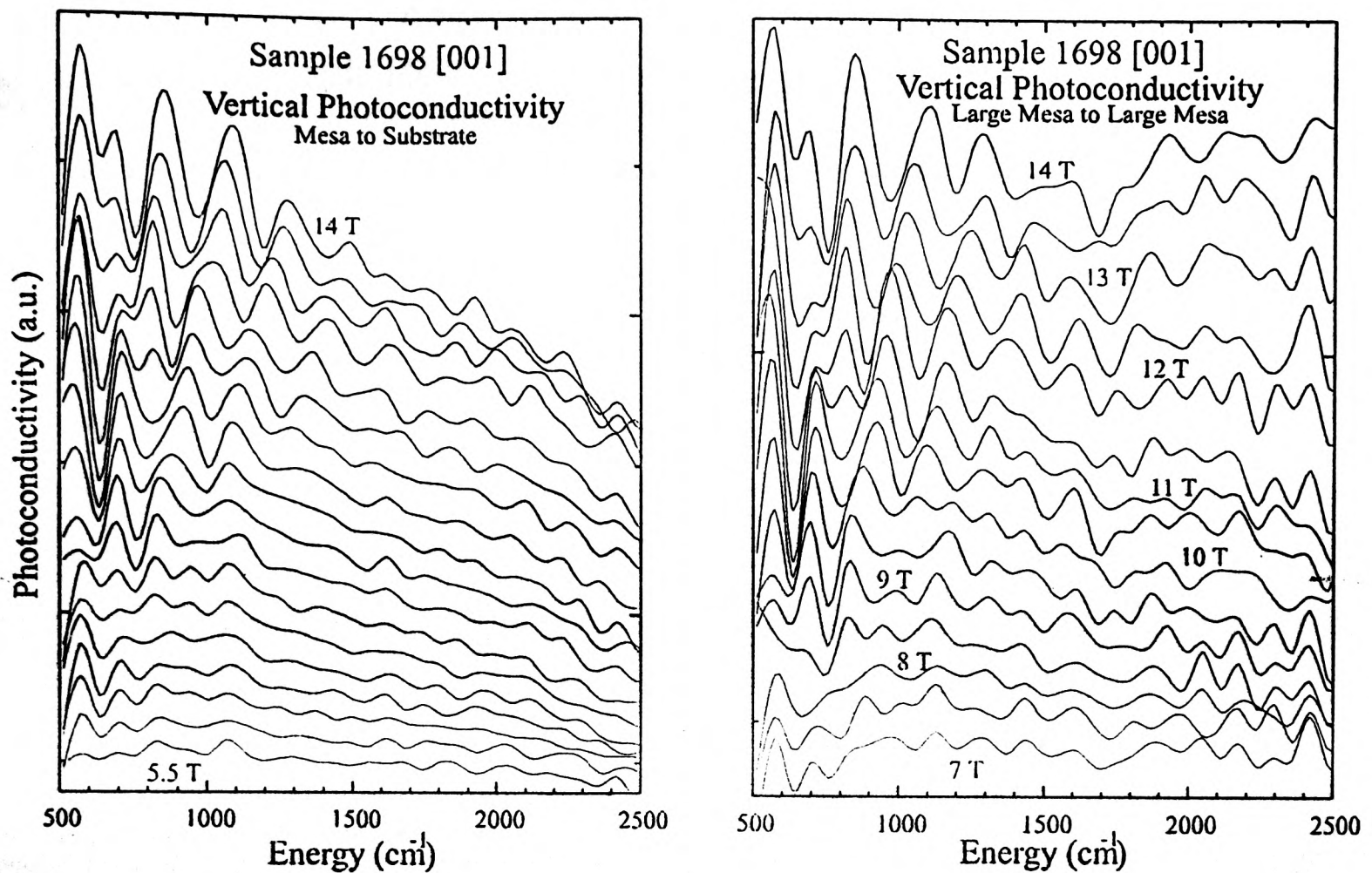


Figure 6.8: Vertical photoconductivity data for sample 1698, for two current paths. The data on the left represents the conductivity of a path between a mesa and the substrate. The data on the right is from a current path between two large mesas. The spectra are ratioed against the zero-field response.

Malcolm Pate of the EPSRC fabrication facility at Sheffield University evaporated gold on the surface of the sample with a mask, to achieve a set of mesas of different size on the surface, to which contacts were made. The sample was deeply etched in other places, giving access to the substrate layer, for the bottom contact. The sample was then glued in a ceramic “holder,” to safeguard the fragile gold contacts. A schematic view is provided in Fig. 6.7.

Again, the standard CR setup was used, with the sample mounted in the Faraday configuration, at 2K in the field center of a superconducting magnet. A Bruker 113v Fourier transform far-infrared spectrometer provided the illumination, and measurements were made by contacting various mesas and substrate regions. This is the origin of the term “vertical” transport, as here excited carriers will flow vertically (in the growth direction), perpendicular to the superlattice layers.

Although not all mesas provide good contacts, in general one is presented with a large number of possible current paths, unlike the lateral photoconductivity set-up. A number of permutations can be attempted, to achieve optimum signal. The most obvious path, from a large or small mesa to the substrate, provided good signal which showed similar structure to the lateral photoconductivity measurements. One can also select a path between two contacts,

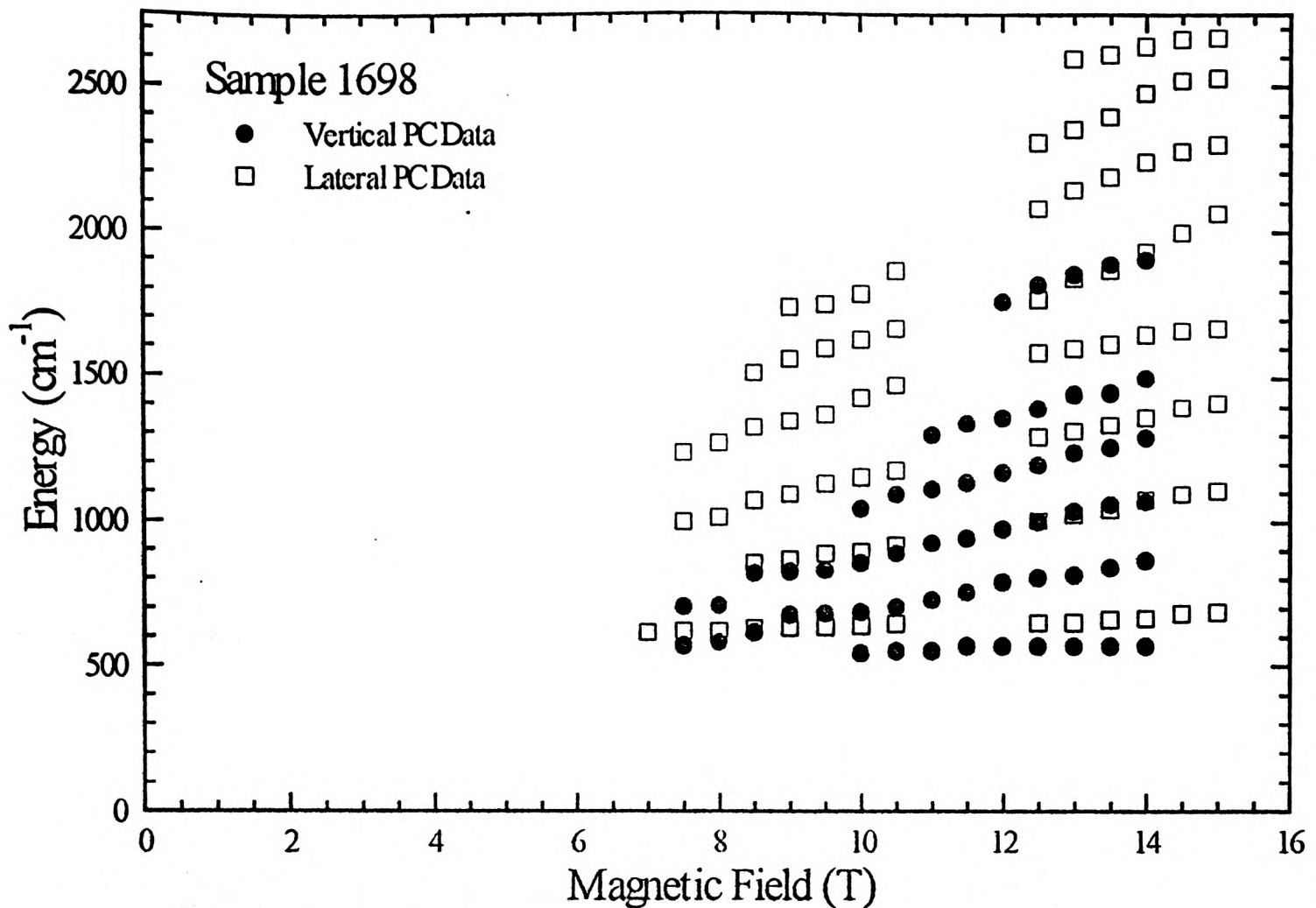


Figure 6.9: Comparison of lateral and vertical photoconductivity measurements.

which requires that the current flow both vertically and horizontally. These mesa-to-mesa current paths also gave strong photoresponse.

6.3.2 Results and Discussion

Fig. 6.8 show typical spectra obtained from the vertical photoconductivity set-up. As before, there is a sharp $n = 0$ band-edge transition around $20 \mu\text{m}$, followed by a series of higher-order interband Landau transitions. As with the lateral photoconductivity spectra of 1698, no spin-splitting or higher-subband transitions are observed. However, the number of transitions and the strength of the response is on a par with the lateral photoconductivity data. This indicates that vertical contacts can provide acceptable response for device applications.

Plotting the resonance positions versus field allows for a comparison of the lateral and vertical photoconductivity measurements (Fig. 6.9). The agreement between the two measurements is acceptable, considering that each is performed on different pieces of the structure, and that in photoconductivity there is some question as to whether peaks or valleys in the conductance actually correspond to quantum transitions. In any case, the extrapolated zero-field band gap is roughly identical in each case.

6.4 Conclusions

In this chapter the photoconductive response of semiconducting InAs/GaSb superlattices was measured. The variation of band gap with layer thickness is found to match theory very well. Contrary to expectations, the InAs/GaSb superlattice system is capable of very long-wavelength band gaps, with strong absorption even for wide layers. Layer fluctuations do have an effect on the sharpness of response; it appears from this data and published results that MBE may be preferable for thin-layer samples, while MOVPE produces better thick-layer (although still semiconducting) structures. Vertical photoconductivity measurements indicate that normal-incidence detection of far-infrared radiation may be achieved with minimal sample processing.

6.5 References

- [1] D. L. Smith and C. Mailhot, *J. Appl. Phys.* **62** (1987) 2545.
- [2] J. H. Roslund and T. G. Andersson, *Super. Micro.* **16** (1995) 77.
- [3] E. R. Heller, K. Fisher, F. Szmulowicz, F. L. Madarasz, *J. Appl. Phys.* **77** (1995) 5739.
- [4] J. P. Loehr, *Appl. Phys. Lett.* **67** (1995) 2509.
- [5] L. L. Chang, N. Kawai, G. A. Sai-Halasz, R. Ludeke, and L. Esaki, *Appl. Phys. Lett.* **35** (1979) 939; L. L. Chang, *J. Phys. Soc. Japan* **49** (1980) Suppl. A 997; see also the references in Chapter 3.
- [6] H. Sakaki, L. L. Chang, G. A. Sai-Halasz, C. A. Chang, and L. Esaki, *Solid State Comm.* **26** (1978) 589.
- [7] H. Bluyssen, J. C. Maan, P. Wyder, L. L. Chang and L. Esaki, *Solid State Comm.* **31** (1979) 35.
- [8] P. Voisin, G. Bastard, C. E. T. Gonçalves da Silva, and M. Voos, *Solid State Comm.* **39** (1981) 79.
- [9] R. H. Miles, D. H. Chow, J. N. Schulman, and T. C. McGill, *Appl. Phys. Lett.* **57** (1990) 801.
- [10] D.H. Chow, R.H. Miles, J.N. Schulman, D.A. Collins, T.C. McGill, *Semicond. Sci. Tech.* **6** (1991) C47.
- [11] I. H. Campbell, I. Sela, B. K. Laurich, D. L. Smith, C. R. Bolognesi, L. A. Samoska, A. C. Gossard, and H. Kroemer, *Appl. Phys. Lett.* **59** (1991) 846.

- [12] J. P. Omaggio, J. R. Meyer, R. J. Wagner, C. A. Hoffman, M. J. Yang, D. H. Chow, and R. H. Miles, *Appl. Phys. Lett.* **61** (1992) 207.
- [13] J. Katz, Y. Zhang, and W. I. Wang, *Appl. Phys. Lett.* **62** (1993) 609.
- [14] T. C. Hasenberg, D. H. Chow, A. R. Kost, R. H. Miles, and L. West, *Electron. Lett.* **31** (1995) 275.
- [15] E. R. Youngdale, J. R. Meyer, C. A. Hoffman, F. J. Bartoli, R. H. Miles, and D. H. Chow, *J. Vac. Sci. Technol.* **B 12** (1994) 1129.
- [16] E. R. Youngdale, J. R. Meyer, C. A. Hoffman, F. J. Bartoli, C. H. Grein, P. M. Young, H. Ehrenreich, R. H. Miles, and D. H. Chow, *Appl. Phys. Lett.* **64** (1994) 3160.
- [17] C. H. Grein, P. M. Young, and H. Ehrenreich, *J. Appl. Phys.* **76** (1994) 1940.
- [18] C. H. Grein, H. Cruz, M. E. Flatte, and H. Ehrenreich, *Appl. Phys. Lett.* **65** (1994) 2530.
- [19] R. Balcerak, *Semicond. Sci. Tech.* **6** (1991) C1.
- [20] D. M. Symons, *D. Phil. Thesis*, Clarendon Lab, Oxford; and see also the references given in Chapter 1.
- [21] G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, *Phys. Rev. B* **26** (1982) 1974.
- [22] J. Cen and K. K. Bajaj, *Phys. Rev. B* **45** (1992) 14380.

Chapter 7

Modeling

In this chapter I use the envelope function approximation described in Chapter 2 to model the InAs/(Ga,In)Sb system. I first turn to semiconducting (thin-layer) superlattices, the simplest structure to model. Methods of engineering optimal band gap response are discussed. The focus then shifts to semimetallic (thick-layer) structures. The self-consistent calculation is explained, and then applied to a variety of systems. The phenomenon of “band gaps” appearing in semimetallic structures is discussed, and the far-infrared absorption properties of thick-layer structures is assessed. The self-consistent calculation is extended to include magnetic fields, and multi-band self-consistent magnetic field results are presented for the first time.

7.1 MODELING THE INAS/GASB CROSSED-GAP SYSTEM	128
7.1.1 PREVIOUS WORK	128
7.1.2 STRAIN	129
7.1.3 PIEZOELECTRIC FIELDS	132
7.2 SEMICONDUCTING SUPERLATTICES.....	133
7.2.1 EXPLICIT INTERFACE EFFECTS	133
7.2.2 LAYER THICKNESS FLUCTUATION EFFECTS	137
7.2.3 ABSORPTION MODELING: FAR-INFRARED DETECTORS.....	139
7.3 SEMIMETALLIC SUPERLATTICES.....	143
7.3.1 SELF-CONSISTENCY	143
7.3.2 SIMPLIFICATIONS USED IN THE CALCULATIONS	149
7.3.3 "BAND GAPS"	150
7.3.4 FAR-INFRARED INTERBAND DETECTORS.....	153
7.4 MAGNETIC FIELDS IN INTRINSIC SYSTEMS.....	154
7.4.1 SIMPLE MODEL.....	155
7.4.2 MULTI-BAND TREATMENT.....	157
7.4.3 MAGNETIC FIELD TRANSITIONS.....	160
7.5 CONCLUSIONS.....	160
7.6 REFERENCES	160

7.1 Modeling the InAs/GaSb Crossed-Gap System

The InAs/GaSb system is a popular choice for $k\cdot p$ modeling. Part of the reason is the relative maturity of the growth techniques, so that many groups worldwide have access to samples. Another reason is the interesting physics of a type-II crossed-gap lineup, especially when compared to the more common type-I lineup of GaAs/AlGaAs structures.

To date, however, almost all multi-band modeling of this system has focused on semiconducting (thin-layer) samples. This is possibly because the immediate application of InAs/GaSb structures seems to be far-infrared devices, where the crossed-gap allows tuning the band gap to very small energies (long wavelengths). The more likely reason for the lack of studies of semimetallic systems, however, is that modeling thicker layers requires a self-consistent model. Self-consistency is very difficult to implement with multi-band formalisms, because most assume a particular form of the potential *a priori*.

[Note: in this chapter, as in Chapter 2, I use atomic units (see section 1.8)].

7.1.1 Previous Work

From the beginning, it was recognized that the crossed-gap nature of InAs/GaSb structures would require a multi-band treatment. The first papers by Chang and Sai-Halasz [1-3] used both linear combinations of atomic orbitals (LCAO) and two-band $k\cdot p$ methods to determine the band gaps of thin-layer InAs/GaSb superlattices. Semimetallic structures were first investigated with a self-consistent (decoupled) Thomas-Fermi approach [2], which gave reasonable agreement with transport measurements for slightly semimetallic systems. Bastard *et al.* [4] studied excitons in the InAs/GaSb system, and found that due to the separation of carriers, the exciton binding energy was very small, around 1 meV.

In 1983 Altarelli published the first and only self-consistent, multi-band study of the InAs/GaSb system, concluding that even thick-layer superlattices would be zero- or small-gap semiconductors [5]. Voisin *et al.* [6] published a short paper on the difference in interband selection rules between type-I and type-II systems in 1984, and there was little theoretical development of the system until Smith and Mailhot's 1987 paper which predicted that InAs/(Ga,In)Sb superlattices should perform as well or better than the HgCdTe alloy at detecting far-infrared radiation [7].

Since 1987 the theoretical study of the InAs/GaSb system has steadily increased. Much of the latest work concerns the optimization of far-infrared interband detectors [8-11]

and lasers [12], but other groups have also realized the potential of intersubband devices [13], particularly as the strong band-mixing allows for intersubband absorption of normally incident light.

The work here will add to the general study of semiconducting systems. My results confirm the recent work on absorption optimization [10,11], and also suggest a way to decrease the detrimental effects of layer fluctuations. The primary contribution of this chapter, however, is the study of semimetallic systems. I extend Altarelli's early work to thicker layers, and discover some indirect negative band gap structures. In addition, I find a startling result which perhaps could have been predicted from Altarelli's band structure: semimetallic superlattices could make *much* better far-infrared detectors than semiconducting superlattices.

7.1.2 Strain

InAs and GaSb are nearly lattice-matched materials (lattice constants are 6.058 Å for InAs, 6.095 Å for GaSb). InAs/GaSb structures may be grown to almost any thickness without significant dislocations, and the modeling of such systems does not normally require a treatment of strain effects. However, as was pointed out by Smith and Mailhot in 1987, the surest way to improve absorption in an InAs/GaSb superlattice is to make the layers as thin as possible, and for a given band gap that requires the addition of indium to the barrier. Because the lattice constant of InSb is so large (6.479 Å), the inclusion of only 5-10% indium in the barrier is enough for the strain to affect the electronic structure significantly. Warburton [14], Pikus and Bir [15], and Van de Walle [16] all give excellent descriptions and theoretical derivations of how strain should be handled in a multi-band formalism. Here I will show how I have included the effects of strain in my modeling.

I assume that the lattice parameter in the plane of the superlattice layers is constant through the structure. This parameter can be the lattice constant of the buffer layer (usually GaSb), while for free-standing, many-period superlattices it is a weighted average of the lattice constants of the different layer materials. In any case, when modeling these structures a value of a_G (the in-plane lattice constant) is taken as an input. The well layers (InAs) will always be under tension, as both the buffer layer of GaSb and free-standing superlattices will have a lattice constant $a_G > a_{InAs}$. The barrier layers of (Ga,In)Sb will usually be under compression, although obviously GaSb layers grown on a GaSb buffer layer will be unstrained.

In Chapter 2 I derived a formalism for 8-band $k \cdot p$ Hamiltonians in arbitrary growth directions, and Los *et al.* [17] derive expressions for the strain tensor in arbitrary directions.

Here I use results for the two most symmetric directions, [001] and [111], as these are the growth directions commonly used by the growers at the Clarendon. For each layer the in-plane strain $\epsilon_{\parallel}$ is calculated as

$$\epsilon_{\parallel} = \frac{a_G}{a} - 1, \quad (7.1)$$

where a is the unstrained lattice constant of the layer material. The growth-direction strain $\epsilon_{\perp}$ is related to the in-plane strain by

$$\epsilon_{\perp} = -D_{\alpha} \epsilon_{\parallel}, \quad (7.2)$$

where D_{α} is an orientation-dependent parameter [16], given by

$$\begin{aligned} D_{[001]} &= 2 \frac{C_{12}}{C_{11}}, \\ D_{[111]} &= 2 \frac{C_{11} + 2 C_{12} - 2 C_{44}}{C_{11} + 2 C_{12} + 4 C_{44}}, \end{aligned} \quad (7.3)$$

where the C_{ij} 's are the elastic coefficients of the layer material. The growth-direction lattice constant is then given by $a_{\perp} = a (\epsilon_{\perp} + 1)$. Then the change in volume of the primitive lattice cell due to strain (to first-order) is given as

$$\frac{\Delta \Omega}{\Omega} = 2 \epsilon_{\parallel} + \epsilon_{\perp}. \quad (7.4)$$

Pikus and Bir [15] calculated the effects of strain within the $\mathbf{k} \cdot \mathbf{p}$ formalism. Retaining terms to first-order in strain and second-order in k , for the [001] and [111] orientations the strain introduces new constants in the Hamiltonian, of the form

$$\begin{array}{c} c \\ hh \\ lh \\ so \end{array} \begin{pmatrix} C & 0 & 0 & 0 \\ 0 & K_1 + K_2 & 0 & 0 \\ 0 & 0 & K_1 - K_2 & \sqrt{2} K_2 \\ 0 & 0 & \sqrt{2} K_2 & K_1 \end{pmatrix}, \quad (7.5)$$

where the bands feel the effects of hydrostatic strain

$$\begin{aligned} C &= a_c \frac{\Delta\Omega}{\Omega}, \\ K_1 &= a_v \frac{\Delta\Omega}{\Omega}, \end{aligned} \quad (7.6)$$

and shear strain

$$\begin{aligned} K_2^{[001]} &= 2b(\epsilon_{\parallel} - \epsilon_{\perp}), \\ K_2^{[111]} &= \frac{2}{\sqrt{3}}d(\epsilon_{\parallel} - \epsilon_{\perp}), \end{aligned} \quad (7.7)$$

where a_c and a_v are the conduction and valence band hydrostatic deformation potentials, and b and d are the tetragonal and rhombohedral deformation potentials, respectively. The effects of strain are shown schematically in Fig. 7.1. In short, for most materials tension acts to reduce the band gap of the material, while compression will increase the band gap.

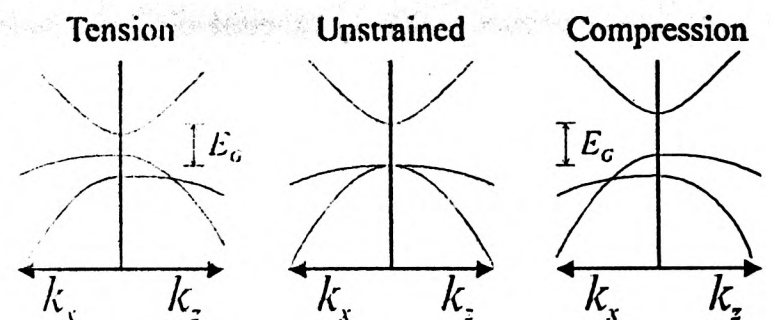


Figure 7.1: The effects on strain on the band-edge energies. For the cases of tension and compression, the unstrained band-edges and gap are given.

It is not obvious how one determines the band lineups of different materials under strain, since the conduction and valence bands move in all directions. Van de Walle and Martin [18] and Van de Walle [16] have determined that the offset of the “average” valence band-edge (the average of the heavy- and light-hole edges) is strain-independent, and I use that assumption here, as have authors before me [7-10] (see Fig. 7.2).

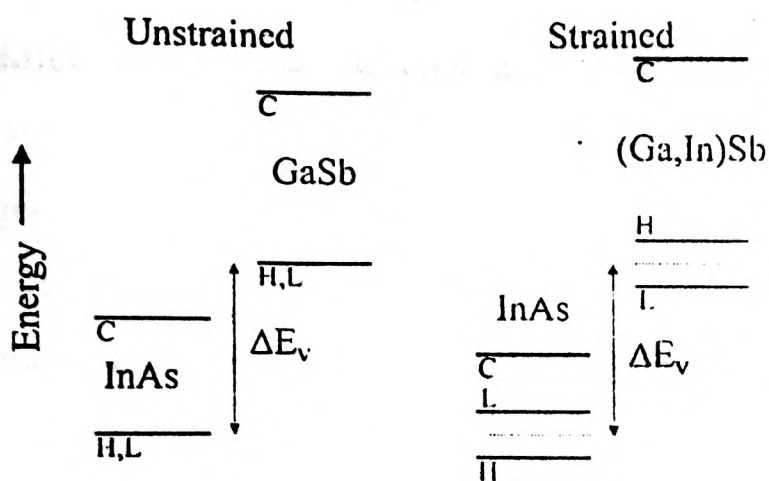


Figure 7.2: Band-edge lineups of strained materials. Although strain moves the band edges, the “average” valence band offset ΔE_v remains constant.

The benefit of a strained InAs/GaSb system is obvious in Fig. 7.2: although the valence band offset is the same, the band overlap (the difference between the GaSb heavy-hole edge and the InAs conduction edge) increases dramatically with strain. This means that for a given band gap, the layers of a strained system will be much thinner than those of an unstrained system, leading to enhanced optical matrix elements [7].

7.1.3 Piezoelectric Fields

In some crystal orientations, strain can induce electric fields in the structure, as well as move the band edges. For strained non-[001] orientations, it has been shown by Smith [19] that the deformed shape of the primitive zincblende cell allows for a nonzero polarization, and this leads to an electric field which is maximum for the [111] orientation. The field arises from non-zero off-diagonal elements in the strain tensor. For [001] structures, no off-diagonal strain elements arise [19,20], but for [111] structures, off-diagonal strains occur and are related to the in-plane strain by

$$\varepsilon_{xy} = \frac{C_{11} + 2C_{12}}{4C_{44}} \varepsilon_{\parallel}, \quad (7.8)$$

where ε_{xy} is the off-diagonal strain term. The total piezoelectric field within the material is then given by [20]

$$E_{pz} = - \frac{4 \pi \sqrt{3} e_{14} \varepsilon_{xy}}{\varepsilon_s}, \quad (7.9)$$

where e_{14} is the piezoelectric constant and ε_s is the dielectric constant of the material. Therefore, for a superlattice grown in the [111]-orientation, the piezoelectric field in each layer may be calculated using Eq. (7.9). Since the off-diagonal strain term varies with the in-

plane strain, the piezoelectric field will point in different directions, depending on whether the layer is under tension or compression. In general, the piezoelectric fields in different layers will not cancel, leading to a net field across a superlattice period. It is assumed that carriers redistribute outside the superlattice to cancel the macroscopic field [19,20].

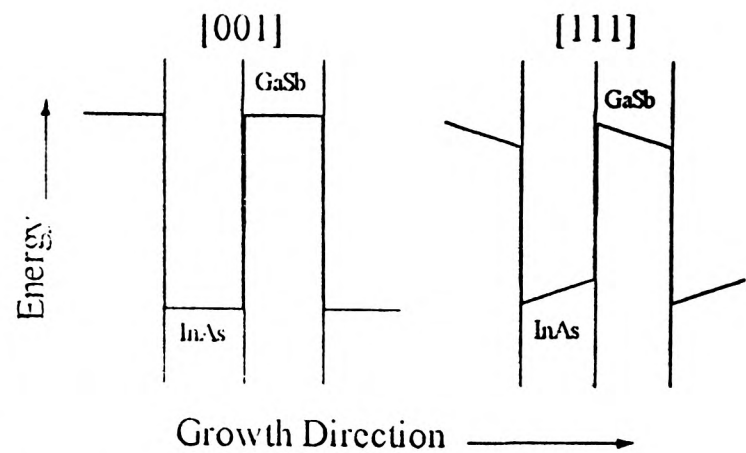


Figure 7.3: The piezoelectric field in an InAs/GaSb superlattice, grown on a GaSb buffer layer. The layer thicknesses are 60 Å.

Fig. 7.3 shows the calculated piezoelectric field in an InAs/GaSb superlattice, grown on a GaSb buffer (so $a_G = 6.095$ Å). Even with no indium in the barrier, the slight lattice mismatch between the two layers ($\Delta a/a \sim 0.6\%$) leads to a piezoelectric field of almost 4×10^4 V/cm. Fields on the order of 10^5 V/cm or more can result from the inclusion of indium in the barrier.

7.2 Semiconducting Superlattices

In this section I study semiconducting superlattices, thin-layer InAs/GaSb systems where no intrinsic charge transfer has occurred. Although the previous decade has produced numerous studies of semiconducting superlattices [7-11], there are still a few points which need addressing: the effects of interface type on the electronic structure, methods of alleviating layer fluctuations, and absorption modeling.

7.2.1 Explicit interface effects

For all of the experimental and theoretical studies of the InAs/GaSb system, accurate values of the band overlap have yet to be determined. At the moment, the band overlaps appear to depend on the interface type (InSb or GaAs), pressure, indium concentration in the barrier, growth orientation, and even growth order (*i.e.*, InAs $\rightarrow$ GaSb or GaSb $\rightarrow$ InAs) [20-25]. Here I model the interfaces explicitly as monolayers (~ 3 Å thick), a thin layer of GaAs or InSb sandwiched between the InAs and (Ga,In)Sb layers. This sort of many-layer-per-period superlattice is difficult to model using transfer-matrix techniques, as the large spurious solutions tend to “wash out” the smaller physical solutions after the many required transfer matrix multiplications.

For this section I use band offsets slightly modified from those provided by Van de Walle [16] (see Table 7.1). In his paper, Van de Walle applies model solid theory, which

Table 7.1: Band offsets, modified from Van de Walle's values [16]. ΔE_v is the valence band offset (so in going from InAs to GaAs, the valence band edge drops by 278 meV). Note that for InAs $\rightarrow$ GaSb, $\Delta E_v = 538$ meV, regardless of interface type.

Materials	ΔE_v (meV)	Materials	ΔE_v (meV)
InAs $\rightarrow$ GaAs	-278	InAs $\rightarrow$ InSb	+709
GaAs $\rightarrow$ InAs	+278	InSb $\rightarrow$ InAs	-709
GaSb $\rightarrow$ GaAs	-816	GaSb $\rightarrow$ InSb	+171
GaAs $\rightarrow$ GaSb	+816	InSb $\rightarrow$ GaSb	-171

allows for the calculation of band structure with respect to an “absolute” energy scale, to calculate the band offsets between different semiconductor structures. His theory also allows for strain, and so he is able to calculate the deformation potentials for each material. The point of using Van de Walle’s offsets is that the band overlap between InAs and GaSb is constant, regardless of interface type. This means that any difference in electronic structure will be due to the physical characteristics of the interface layers. When strain is included the InAs conduction band drops by almost 30 meV, so that Van de Walle’s offsets result in a band overlap of 175 meV, much larger than is predicted by optical or transport experiments. Therefore I modify the offsets to compensate, yielding an interface-type-independent band overlap of approximately 145 meV (depending on the strains in the system).

A note should be made of the suitability of the envelope function approximation (EFA) to modeling these thin layers. In the derivation, it is required that the Fourier components of the envelope functions lie within the first Brillouin zone of the crystal and that the band-edge potential is “smooth” [26,27]. At first glance, the drastic band-edge jumps resulting from 3 Å interface layers seem to completely invalidate the EFA approach. However, in the momentum-matrix technique, the wave functions couple strongly only with those Fourier terms in the potential which are

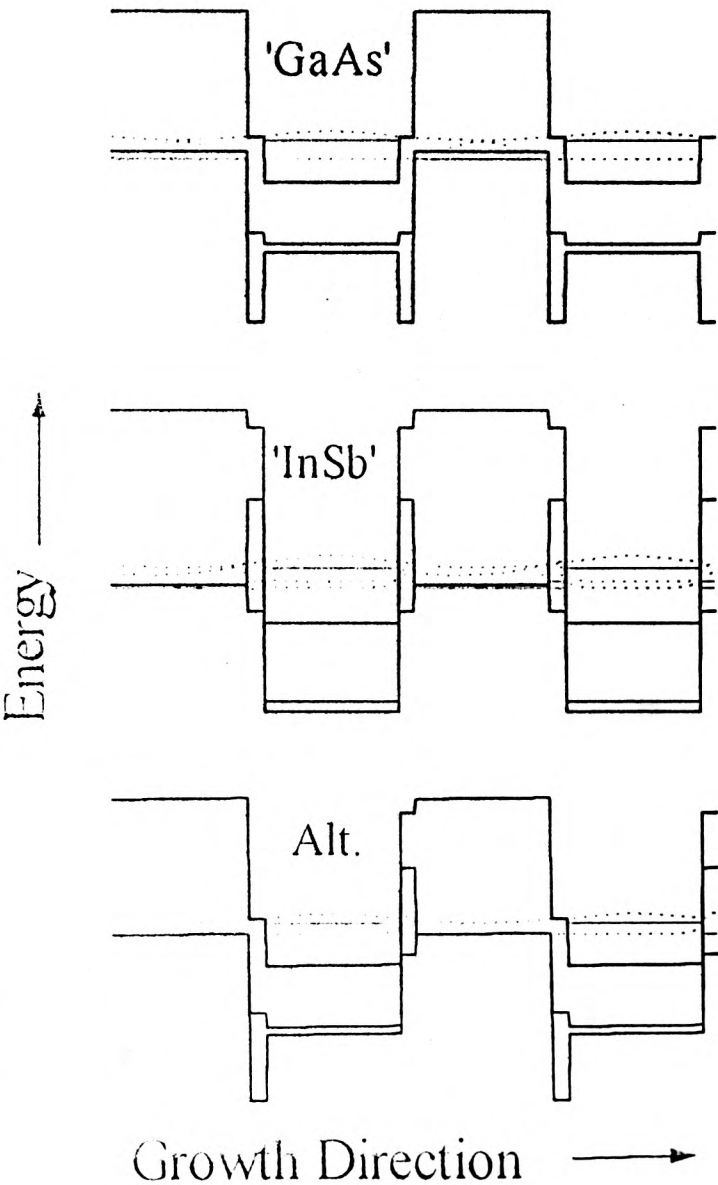


Figure 7.4: Explicit modeling of the interface layers. At the top, GaAs-like interfaces. In the middle, InSb-like interfaces. At the bottom, alternating interface type. All structures are assumed to be grown on a GaSb substrate.

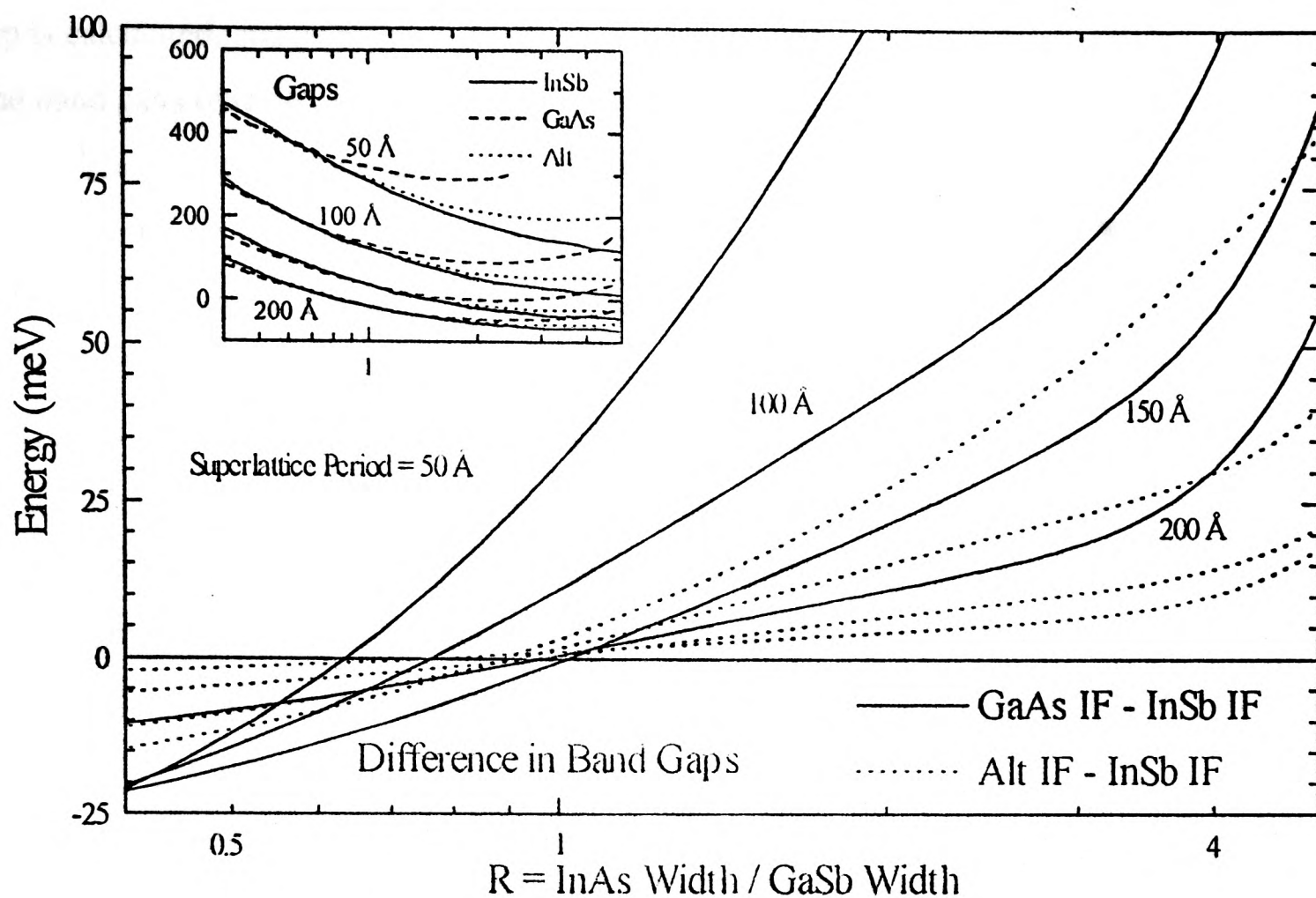


Figure 7.5: Difference in band gaps resulting from explicit interface modeling. The actual calculated band gaps are inset. The effects of interface type are compared relative to the band gaps calculated with InSb-like interfaces. It is seen that $R > 1$ structures grown with GaAs-like or alternating interfaces have larger band gaps than those grown with InSb-like interfaces, although here the actual band overlap between InAs and GaSb is kept constant at 145 meV for all interface types.

close to its own: *i.e.*, high frequency terms in the Fourier expansion of the potential only affect the wave function if it also contains high frequency terms (this is true in any EFA formulation, but the momentum-matrix technique brings out the coupling explicitly). So long as the wave functions contain only low frequency terms, we can disregard the high frequency components of the potential. The conclusion is that we expect the results to be reasonably valid until the wave functions become localized in the interfaces (strong high frequency components). Because of the high strain in the interface layers, and the obvious question of whether a 3 Å layer can be treated as bulk, I am not aiming for quantitative results, but merely qualitative behavior.

The superlattices are therefore modeled with 3 Å interface layers. I test three different cases: InSb-like interfaces, GaAs-like interfaces, and alternating interfaces (one InSb-like and one GaAs-like). The large strains in each interface layer ($\Delta a/a \sim 8\%$) split the valence edge considerably, and move the conduction edge (see Fig. 7.4). For each case, a superlattice thickness d is chosen (from 50 to 200 Å), and the ratio of the layer widths is varied. The band

gap is calculated, and although for large d some gaps are negative I disregard self-consistency. The band gaps obtained from superlattices with different interfaces are then compared.

The result is shown in Fig. 7.5, where several qualitative results are evident. First and most importantly, for superlattices with $R \geq 1$ (InAs at least as thick as GaSb), both GaAs-like and alternating interfaces give band gaps larger than InSb-like interfaces. This indicates that for $R \geq 1$ the “effective” band overlap of InSb-like interfaces is larger than that of GaAs-like or alternating interfaces, in agreement with transport [20] and optical [25] experiments. As expected the difference between effective overlaps is greatest between InSb- and GaAs-like interfaces, with alternating interfaces somewhere in between.

Second, the difference in effective overlaps is greater as R is increased (thicker InAs layers). The superlinear behavior at large R is probably not accurate, since here the thin GaSb layers result in increasing localization of the heavy hole state in the interface layer. But for modest R , we expect the difference in effective overlaps to increase as the well width is increased.

And finally, the difference between effective overlaps decreases with increasing superlattice period. Intuitively, this makes sense, as electrons in very wide layers will feel little or no influences from the interface. Although differences in band overlaps have been calculated from transport results in very thick layers [20], these are cases where $R \gg 1$, where the difference in effective band overlap is expected to be greatest (hence observable even for wide layers). Also, when self-consistent effects are included the bound states move closer to the interfaces, so that quantizing effects of interface layers will still influence the system.

The interface-dependent band overlap is a crucial parameter in predicting device performance. However, when heterostructure band structure is *not* considered and only the fundamental crystal energy states are examined, both theory [16] and experiment [28] agree that the actual band overlap is *independent* of interface type. When an interface-dependent band overlap is discussed, one is therefore implicitly referring to the extra quantization effects of the interface, rather than an actual shifting of the InAs or GaSb bulk band edges relative to the vacuum. This sort of effective band overlap is very useful in modeling, as explicit interfaces are difficult to include in transfer-matrix methods, and are of dubious validity even in more general methods.

The results here show that much previous work on band overlaps can be reproduced with a constant band overlap, with the difference in effective band overlaps arising purely from

the quantizing effects of the interface layer. Therefore, in the interests of simplicity, I use effective band overlaps for the rest of the calculations, and do not model interfaces explicitly. However, it should be remembered that there is in general no reason to suppose that the effective band overlaps will be independent of layer thickness, strain or any other external variables.

An analogous calculation for the [111] case has been performed, but here the strain has even more drastic effects upon the interface layers, and the hole wave functions become localized within 3 Å. Therefore, even the qualitative results are questionable, although they roughly agree with the [001] results presented above. When explicit modeling of interface layers is dropped, and only effective band overlaps are used between InAs and GaSb layers, we find that strain effects alone account for observed differences in [001] and [111] band overlaps [22]. It therefore appears that the band lineup of InAs and GaSb is independent of both interface type and growth orientation.

7.2.2 Layer thickness fluctuation effects

One of the problems facing growers of epitaxial layers is thickness fluctuations. Particularly when growing thin-layer, semiconducting superlattices, a few monolayers error in a layer can shift the band gap by tens of meV. Even under optimal growth conditions, growers can expect errors on the order of a monolayer to occur at different points in the superlattice. However, even with layer fluctuations the average superlattice period tends to remain constant [29]. This is also called “step bunching,” again where thickness fluctuations in one layer are compensated by corresponding fluctuations in a neighboring layer, leading to a superlattice period which remains roughly constant. For devices, then, one would like to find an optimum set of layer thicknesses such that layer fluctuations have minimal effect on the band gap. For this I calculated the band gap for a range of layer thicknesses, where the total superlattice period is kept constant.

The calculation results are presented in Fig. 7.6. For a range of superlattice periods, there is an obvious band gap extremum at $R \sim 2.5$, where R is the ratio of the InAs and GaSb layer widths. The band gap of a structure grown with thick InAs layers is therefore expected to be relatively insensitive to layer fluctuations, as has been predicted before by transfer-matrix methods [30].

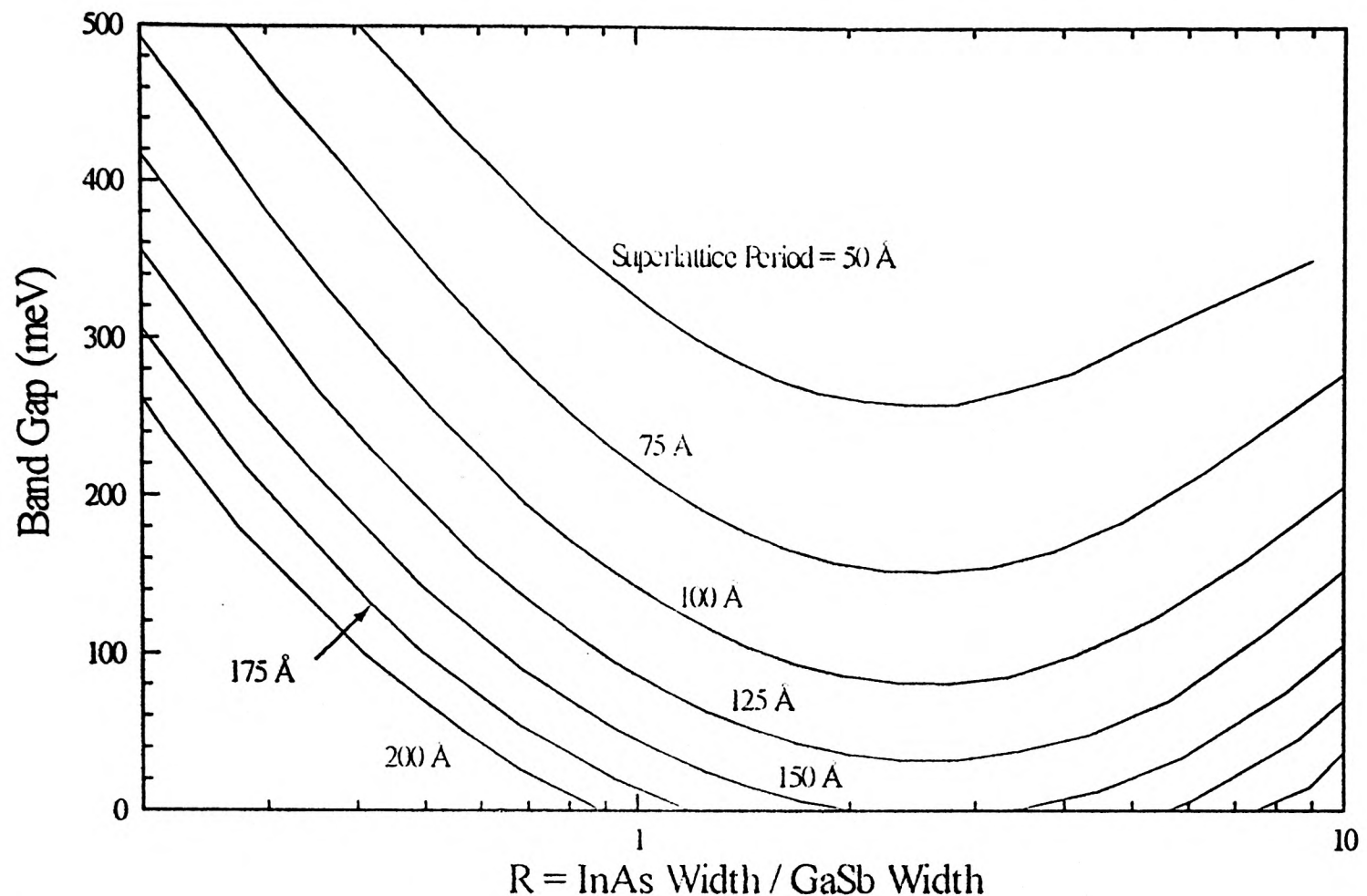


Figure 7.6: Band gap variation with the layer width ratio. For all superlattice periods, a minimum occurs at the ratio $R \sim 2.5$.

Since the extremum position is actually a minimum, a further benefit of growing $R \sim 2.5$ structures is that for this ratio of InAs thickness, the band gap is minimized. This means that for a given band gap, the superlattice has the thinnest possible layers. Since thinner layers result in increased wave function overlap, strongest absorption for a given band gap is expected at $R \sim 2.5$.

To check this result, the optical matrix element of the ground electron and heavy hole bound states has been calculated at $k_{\parallel} = 0$ (k is the momentum in the plane parallel to the growth layers):

$$|M|^2 = \frac{P^2}{2} |\langle f_{eo}(k_{\parallel} = 0) | f_{ho}(k_{\parallel} = 0) \rangle|^2, \quad (7.10)$$

where P is the Kane matrix element, and f_i is the envelope function of the i th subband. This expression for $|M|^2$ is derived from the general expression in Chapter 2 (see also Eq. (7.11) below). Here I assume light polarized in the plane of the layers (*i.e.*, normally incident light).

The results of the matrix element calculation are presented in Fig. 7.7. As expected, the matrix element for a given band gap is maximized for a choice of $R \sim 2.5$. This agrees well with the results of Smith and Mailhot, who found a similar matrix-element dependence for

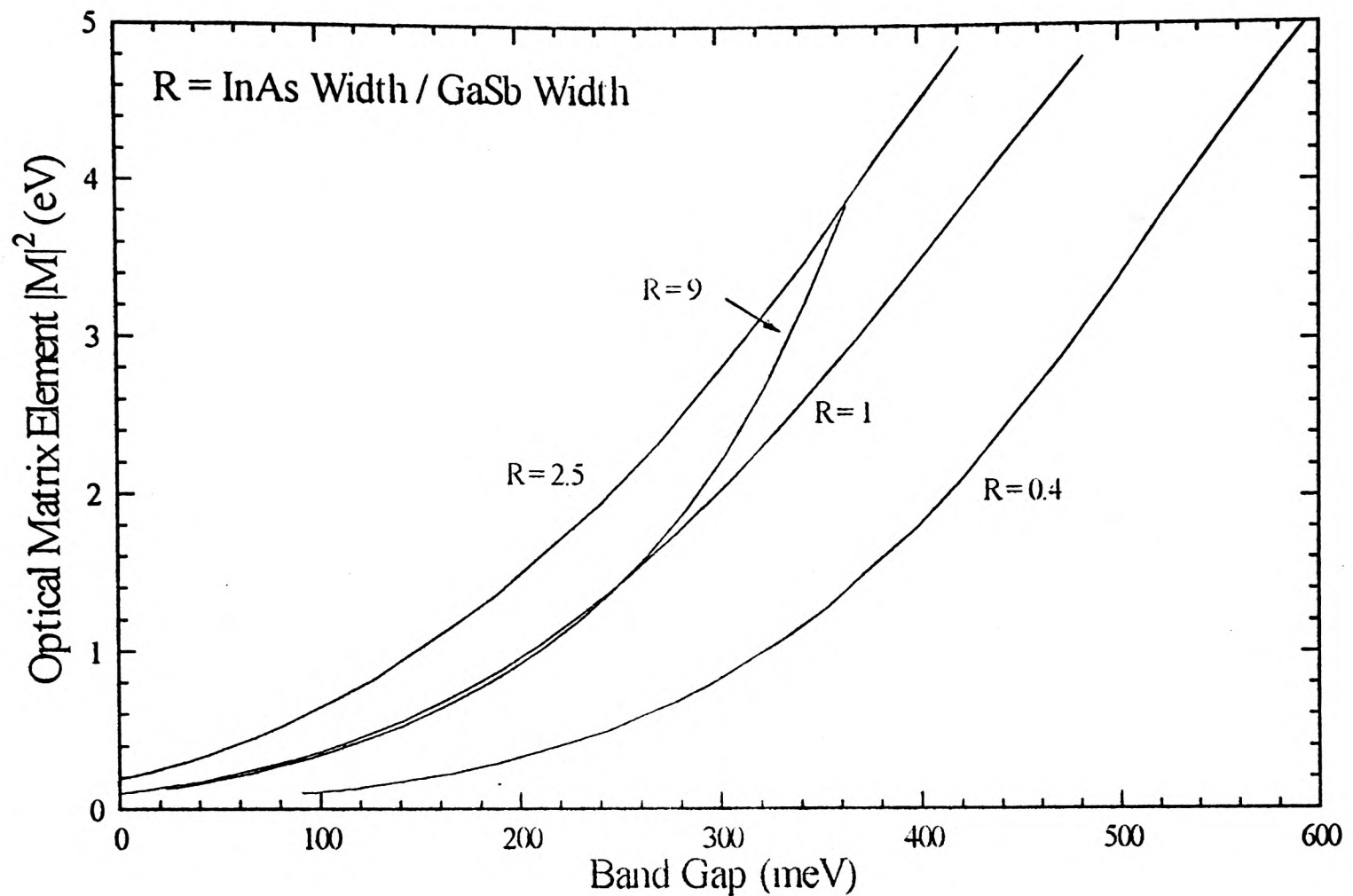


Figure 7.7: Calculated optical matrix element as a function of band gap. The layer thickness ratio $R \sim 2.5$ provides the maximum wave function overlap for all band gaps.

[111] InAs/(Ga,In)Sb superlattices, although they did not attribute the effect to a minimization of the layer widths [7]. The seeming advantage of the $R = 9$ ratio for large band gaps is not technologically feasible, as a superlattice grown with this ratio at a band gap of 300 meV would have a barrier width of 1 monolayer of GaSb (6 Å).

The conclusion, therefore, is that semiconducting superlattices grown with an InAs/GaSb ratio of 2 or 3 to 1 should exhibit optimum optical response, in addition to being the least sensitive to layer fluctuations. Why should a ratio of 2.5 in particular be so insensitive to fluctuations? The most likely explanation lies in the difference between the masses and band coupling of the electrons and heavy holes: electrons are much more sensitive to layer fluctuations, hence need a large layer to reduce the effects of monolayer variations. Although I will claim that optimum absorption is actually achieved with semimetallic structures, the general result found here is expected to hold for thick-layer superlattices as well: thick InAs layers (relative to the GaSb layers) result in a band gap least sensitive to layer fluctuations.

7.2.3 Absorption Modeling: Far-Infrared Detectors

In previous studies of the semiconducting InAs/GaSb system for far-infrared devices, the interband optical matrix element at the Γ point $|M|^2$ has been the chief figure of merit when comparing different structures [7,9-11]. As such, it is probably a decent measure of the absorption of the system, as the wave function overlap appears to be the dominant concern when designing thin-layer structures, and most overlap information is contained in $|M|^2$. In addition, the joint-density-of-states (defined below) is usually a maximum at the Γ point.

However, most absorption actually occurs away from the Γ point, where $k_{\parallel} \neq 0$. Also, although two structures may share similar matrix elements, their energy band dispersions may lead to radically different joint-density-of-states, and so different absorption. Detailed comparison of different structures, and comparison with experiment, often requires inclusion of the $k_{\parallel}$ -dispersion when calculating absorption.

The general expression for absorption (expressed as absorption per superlattice period per unit illuminated area), repeated from Chapter 2, is

$$\alpha(\omega) = A \sum_{i,f} |\langle i | \epsilon \cdot p | f \rangle|^2 \delta(E_f - E_i - \omega) [f(E_i) - f(E_f)], \quad (7.11)$$

where

$$A = \frac{4 \pi^2}{n c \omega}, \quad (7.12)$$

where n is the index of refraction, c the speed of light, ω the frequency of incident radiation, i and f refer to the initial and final states of the transition, and $f(E)$ is the Fermi filling factor at energy E . As in Chapter 2, I assume a low-temperature distribution of carriers, and so to account for the third term (filling factors) I restrict the summation to all states i below the Fermi level, and all states f above it. The momentum matrix element $|\langle i | \epsilon \cdot p | f \rangle|$ is solved as discussed in Chapter 2, and so gives rise to selection rules, momentum conservation, and accounts for wave function overlap.

When actually calculating the absorption of a structure, the form of Eq. (7.11) is inconvenient. The standard practice is to convert the sum over states i and f into an integral over $k_{\parallel}$ -space. However, the delta function constraining $\omega = E_f - E_i$ is expressed in terms of

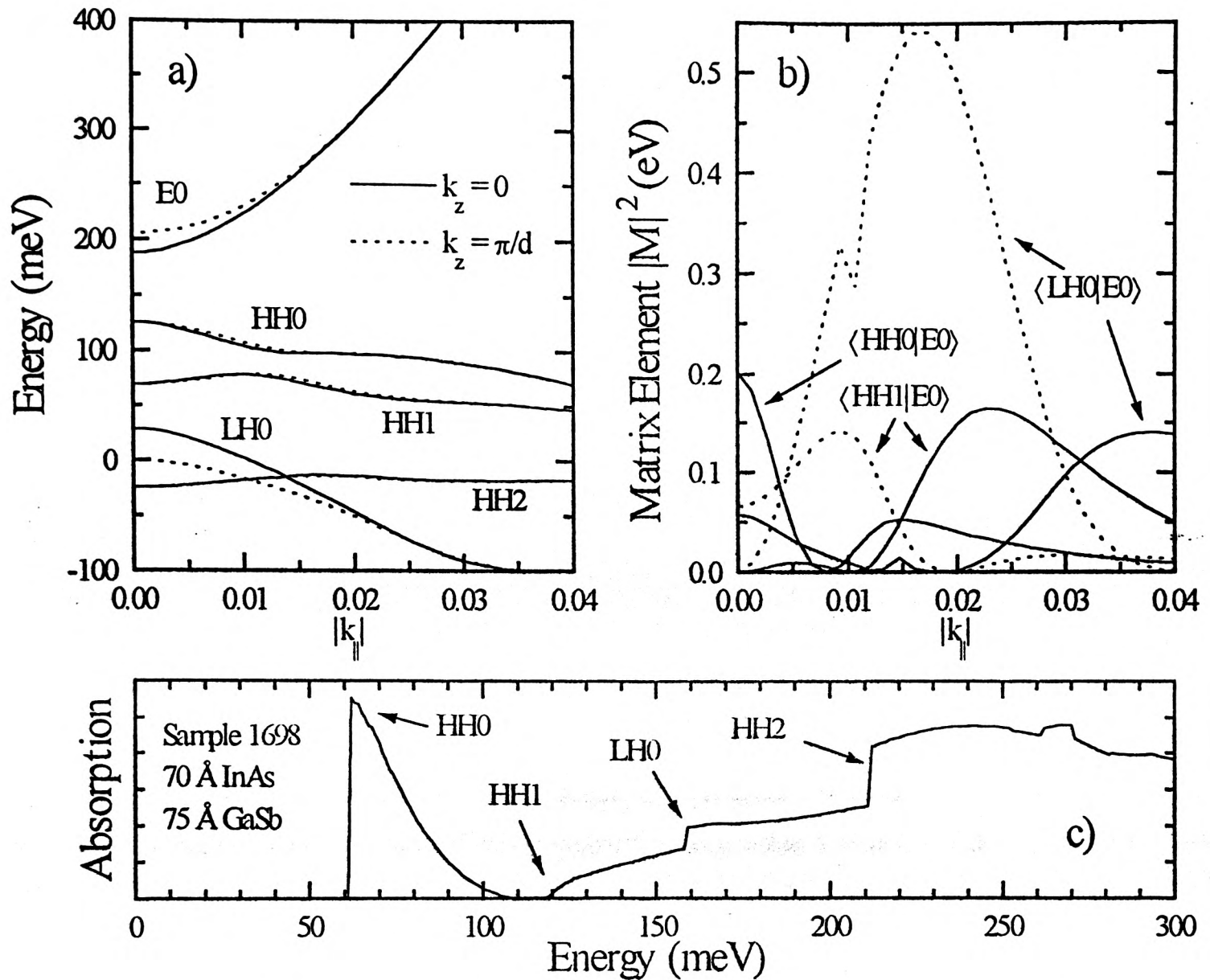


Figure 7.8: An absorption calculation for sample 1698 [001] (70 Å InAs, 75 Å GaSb). In a), the energy band dispersion is calculated. In b), the wave functions at each $k_{||}$ point are used to determine the optical matrix elements $|M|^2$. Finally in c) the energy band separations, curvatures (JDOS), and matrix elements are used to calculate the total absorption spectrum. In c) all transitions have as a final state the lowest conduction band state $E0$, and the initial states are labeled.

energy. A standard mathematical identity is used to convert the delta function to be $k_{||}$ -dependent:

$$\delta(E(k)) = \sum \frac{\delta(k-k_0)}{|\nabla_k E|_{k_0}}, \quad (7.13)$$

where the sum is over all values of k_0 such that $E(k_0) = 0$. The final expression for the absorption between two subbands m and n is then

$$\alpha_{mn}(\omega) = 2 \pi A \sum_{k_0} |\langle \Psi_m(k_0) | \varepsilon \cdot p | \Psi_n(k_0) \rangle|^2 \frac{|k_0|}{|\nabla_k (E_m - E_n)|_{k_0}}, \quad (7.14)$$

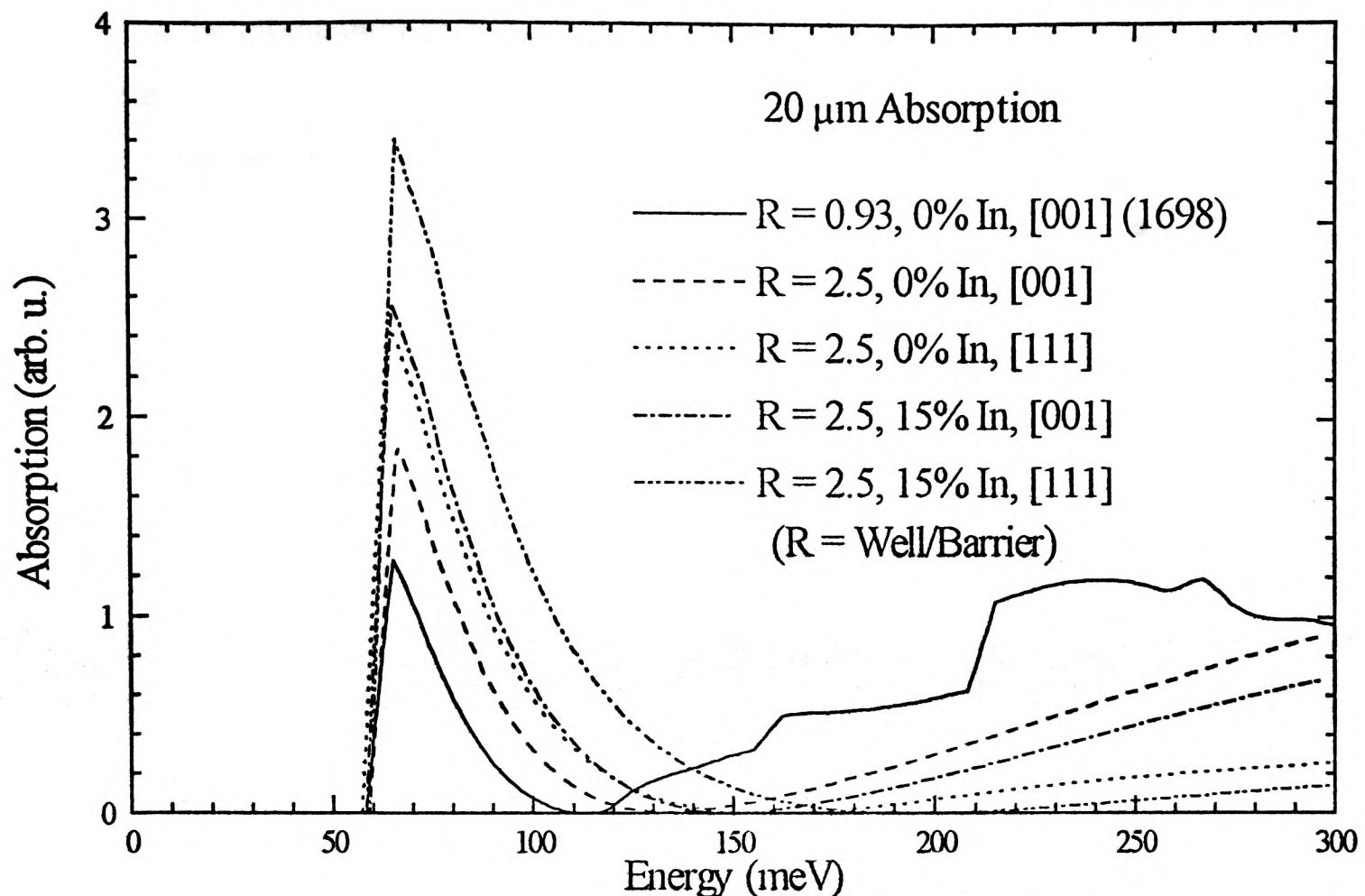


Figure 7.9: A comparison of absorption coefficients of different InAs/(Ga,In)Sb superlattices with a band gap of 62 meV (20 μm). As predicted by Smith and Mailhot, the strongest absorption for a given band gap occurs for [111] structures with indium incorporated into the barrier [7].

where again the sum is over all k_0 such that $\omega = E_m(k_0) - E_n(k_0)$, and the wave function $\Psi_l(k)$ is a combination of envelope and crystal basis functions. The inverse gradient term in Eq. (7.14) is the joint-density-of-states (JDOS). When the energy bands E_m and E_n are parallel, the JDOS is very large. For interband transitions, the electron and hole bands tend to be parallel only at the Γ point, and so that is the dominant contribution to absorption, even though $|k_0|$ (the numerator) is small. The advantage of semimetallic structures (discussed below) is that the bands often become parallel at finite $k_{\parallel}$ values, leading to a JDOS much enhanced over semiconducting values.

In deriving Eq. (7.14) the axial approximation was assumed, where anisotropy in the x - y plane is ignored. The axial approximation leads to important simplifications when constructing Hamiltonians (it allows for block-diagonalization at zero-field, and a simple form with magnetic field), and here simplifies the form of the absorption coefficient (the gradient term is a simple one-dimensional derivative). The axial approximation is expected to hold for small values of $k_{\parallel}$, where anisotropy is weak. For the large values of $k_{\parallel}$ where anisotropy becomes more important, the JDOS is usually small. Even in the worst case, where anisotropy and the JDOS are both large, the result is only a smearing-out of transitions (see [31] for a comparison of matrix elements calculated along [100] and [110] directions).

Using the momentum-matrix technique, the energies of an InAs/(Ga,In)Sb superlattice are calculated for a discrete series of $k_{\parallel}$ values. At each $k_{\parallel}$ point, the wave functions are used to calculate the momentum matrix element. The transitions between all subbands are examined, and for each photon energy ω the absorption contributions are summed using Eq. (7.14). The energy bands and matrix elements are interpolated quadratically between calculated $k_{\parallel}$ -points.

7.3 Semimetallic Superlattices

As was mentioned in the introduction, there has been only one theoretical study of the semimetallic InAs/(Ga,In)Sb system: Altarelli's 1983 paper [5]. There he found that for a wide range of superlattice periods (although he quotes no numbers), the superlattices were all either zero- or small-gap, that is, although charge transfer had occurred the structure was basically a semiconductor. Using the momentum-matrix technique, I find I reproduce Altarelli's results for thin-layer superlattices ($d < 300 \text{ \AA}$ or so). For thicker layers, however, I find indirect negative band gaps. It is these indirect gaps which then allow semimetallic behavior, where carriers at the Fermi level have access to a large number of empty states for scattering.

7.3.1 Self-Consistency

The defining feature of semimetallic InAs/(Ga,In)Sb superlattices, for the modeler, is that they require self-consistency. Charge transfer from hole to electron states leads to such a large number of carriers ($n_s > 10^{10} \text{ cm}^{-2}$) that Coulombic band-bending terms need to be included in the calculations. The fundamental algorithm of any self-consistent calculation is as follows:

- 1) Make an initial guess at the band-edge potential $V(z)$.
- 2) Calculate the band structure (energies $E(k_{\parallel})$ and envelope functions $f(k_{\parallel}, z)$) from the potential $V(z)$.
- 3) Determine the Fermi level from the band structure (plus extrinsic factors such as doping, interface charges, *etc.*).
- 4) Calculate the Coulombic (electrostatic) band-edge potential $V(z)$ from the band structure and Fermi level.
- 5) Return to step 2) until suitable convergence is obtained.

7.3.1.1 Step 1: Initial guess at the band-edge potential

In many systems, particularly GaAs/AlGaAs heterojunctions, it has been shown that a good initial guess at $V(z)$ can speed convergence (and in fact, a poor guess can sometimes make convergence extremely difficult). Surprisingly, I make no guess at all, that is, I set $V(z) \equiv 0$ for all z .

There are two reasons for this. First, the quantization in an InAs/(Ga,In)Sb is quite strong. The conduction band well is on the order of 1 eV deep, while the valence band well is over 500 meV. Therefore, somewhat accurate bound states are found even in flatband conditions. Even in this case, however, a guess at $V(z)$ might be expected to speed convergence somewhat. The second reason for setting $V(z) \equiv 0$ is that I have programmed a general model, which does not “know” in advance which material layers will be host to electron states, and which to holes, making a nonzero guess difficult. Even in the worst case, however, I find my lack of initial guess costs no more than three iterations in the self-consistent algorithm, and usually only one iteration or less.

7.3.1.2 Step 2: Calculating the band structure from the potential

This step is by far the most difficult of the self-consistent algorithm, as it requires a technique capable of calculating band structures for arbitrary band-edge potentials. In transfer-matrix approaches this is almost impossible, as the form of the envelope function is assumed *a priori*, and the spurious solutions make wide-layer structures difficult to solve. The effective-mass approximation allows one to solve for the band structure numerically, at the price of losing the multi-band treatment.

Fortunately, the momentum-matrix method is completely general with regard to the potential, and no assumption about the envelope function is made (other than the required Bloch condition). Therefore, given the band-edge potential, the band structure is solved using the momentum-matrix method as described in Chapter 2.

One point concerning Hamiltonians must be made. In zero-field cases, I have used block-diagonalized Hamiltonians (Chapter 2). However, those Hamiltonians are valid only for symmetric structures, and contain information about only one spin state. When calculating the charge density of Eq. (7.20), the explicit shape of the wave functions have an impact on the final form of the Coulomb potential. Therefore, both spin states must be included even for symmetric structures, as opposite spin states although degenerate in energy have different wave functions at finite $k_{\parallel}$. The bound states of the system are calculated using both 4x4

block-diagonalized Hamiltonians, which is four times faster than using the full 8x8 (Altarelli uses both a 3x3 spin-up and a 3x3 spin-down Hamiltonian [5]).

7.3.1.3 Step 3: Calculating the Fermi level

Calculating the Fermi level is an iterative procedure in and of itself. A trial Fermi level is selected, then used to calculate the populations of the heterostructure subbands. The total electron and hole densities are compared, and extrinsic doping and interface effects are included as well. If there is an excess of electrons (Fermi level too high), or an excess of holes (Fermi level too low), then the trial Fermi level is readjusted. Like the self-consistent procedure, the process is iterated until convergence is obtained (although it is orders of magnitude faster than band-structure calculations).

Calculating the band populations requires calculating the two-dimensional density of states (2DOS). Given a two-dimensional plane of height and width L , the number of allowed $k_{\parallel}$ points within a circle of radius $k_{\parallel}$ is

$$N = (L/2\pi)^2 \pi k_{\parallel}^2. \quad (7.15)$$

The 2DOS is then the number of allowed $k_{\parallel}$ points per unit energy per unit area

$$\rho(E) = \frac{1}{L^2} \frac{dN}{dE} = \frac{1}{L^2} \frac{dN}{dk_{\parallel}} \frac{dk_{\parallel}}{dE} = \frac{1}{(2\pi)^2} 2\pi k_{\parallel} \frac{dk_{\parallel}}{dE}. \quad (7.16)$$

For a given electron subband i , the total number of populated states per unit area is then

$$n_i = \int_{\phi} \rho(E) dE = \frac{1}{(2\pi)^2} \int_{\phi} 2\pi k_{\parallel} dk_{\parallel}, \quad (7.17)$$

where the integral is over the set ϕ of all populated states. A similar result holds for hole subbands. The result of Eq. (7.17) is that the total population of a given subband is simply the area of populated states in $k_{\parallel}$ space divided by $(2\pi)^2$. This assumes non-degenerate bands (e.g., spin-degenerate bands would have the density multiplied by two). Given a trial Fermi level, Eq. (7.17) is evaluated for each subband i , and summing over all i gives the total electron and hole populations.

7.3.1.4 Step 4: Constructing the band-edge potential from the band structure

Constructing the band-edge potential can essentially be thought of as accounting for many-body effects within the Hartree approximation [32]. There are a number of many-body effects which one must consider when dealing with a large number of carriers, notably the Coulombic, exchange, and correlation interactions [33,34]. For the purposes of the InAs/GaSb system, I focus only on the electrostatic (direct Coulombic) interactions. Although exchange effects are expected to be large for these carrier densities (where $n_s \approx 10^{12} \text{ cm}^{-2}$), I neglect them. This is mainly due to the fact that exchange and correlation interactions have not been well investigated for two-carrier systems.

The band-edge potential $V(z)$ is a sum of two terms (for our purposes), the “bare” band-edge potential $V_{be}(z)$ and the electrostatic potential $V_{es}(z)$. $V_{be}(z)$ is constructed by taking account of the band-edge discontinuities at interfaces. The electrostatic potential is calculated from Poisson’s equation

$$V_{es}'' = \frac{4\pi}{\epsilon_s} q(z), \quad (7.18)$$

where ϵ_s is the dielectric constant of the material, and $q(z)$ is the charge distribution of the superlattice (here I use $q(z)$ for the real space charge distribution so as not to confuse it with $\rho(E)$, the 2DOS). Eq. (7.18) must be integrated twice to find $V_{es}(z)$, leading to two constants of integration. The first constant corresponds to the choice of external electric field. This must be set to zero for superlattices, for the crucial relation $V(z+d) = V(z)$ to hold, although other heterostructures can be solved for applied fields. The second constant is determined by one’s choice for a zero of energy. I take the conduction band minimum as the energy origin, although it makes no difference to the physics of the problem.

Each superlattice layer is likely to have a different ϵ_s . The dielectric constant in each layer is set to $\bar{\epsilon}_s$, the weighted average dielectric constant of the heterostructure, to avoid complications due to image charges. In practice, most III-V semiconductors have dielectric constants differing only by a few percent, so this is a good approximation.

Having agreed on the method of integrating Eq. (7.18), the charge distribution $q(z)$ of the superlattice must be determined. The 2DOS gives a measure of how many states are populated at a given E , $k_{\parallel}$ point. To determine the charge density in real space the 2DOS is

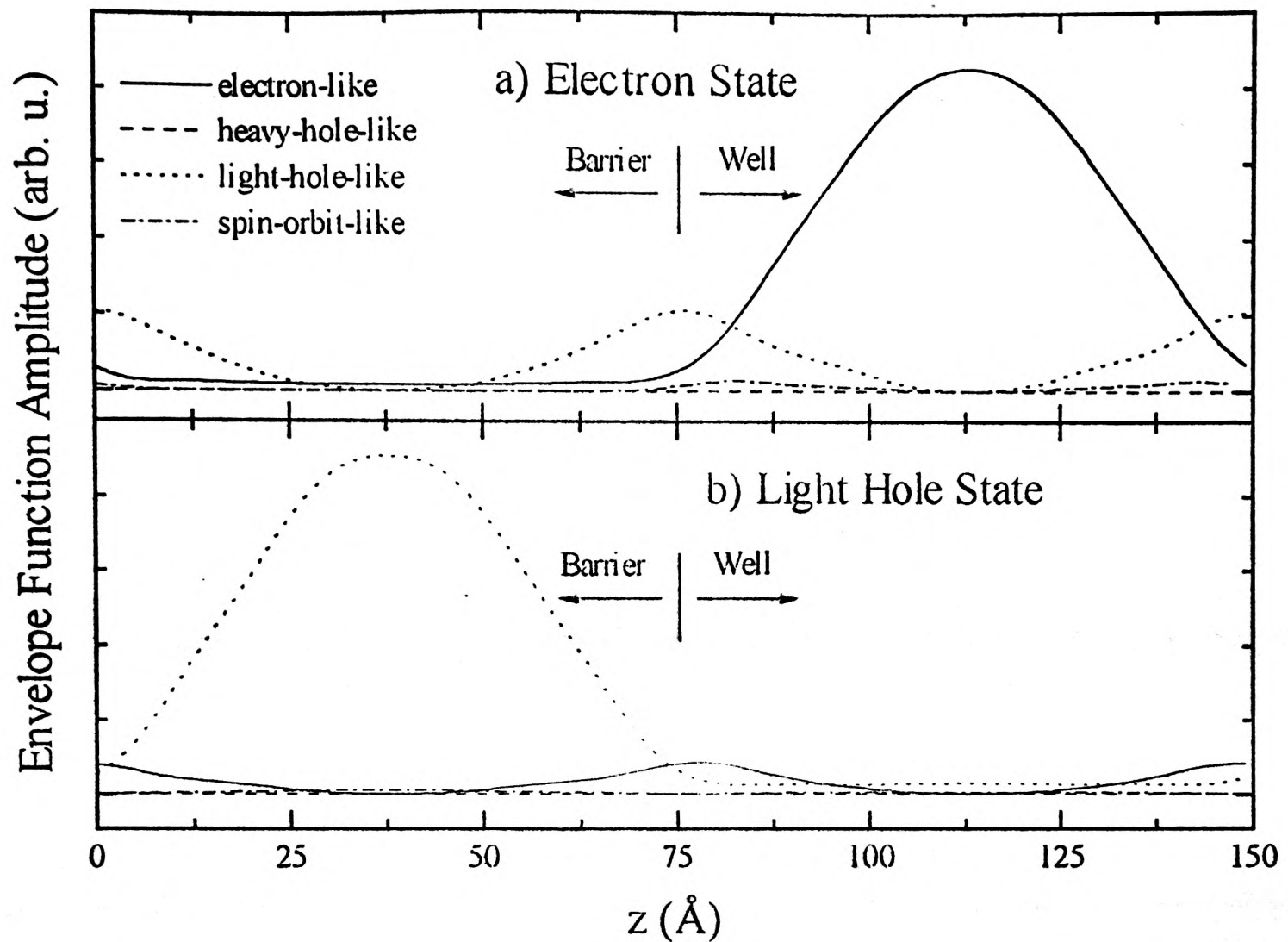


Figure 7.10: The components of the envelope function for an InAs/GaSb superlattice (75 Å InAs, 75 Å GaSb) at $k_{\parallel} = 0$. In a) the envelope function of an electron state is pictured, showing the mixing with light-hole and spin-orbit states. In b) the envelope function of a light-hole state is pictured, showing mixing with electron and spin-orbit states. At $k_{\parallel} = 0$, electron and light-hole states do not mix with the heavy-holes.

modulated by the envelope function. The total envelope function is not used, rather individual band components are used depending on the band populations. For instance, if at a given point the electron states are found to be populated (the band is below the Fermi energy), then the $|s\rangle$ component of the envelope function is used. If the hole states are populated at a given $E, k_{\parallel}$ point then the $|x\rangle, |y\rangle$ and $|z\rangle$ components are used. (See Fig. 7.10, and reference [5])

The total expression for the charge density within a heterostructure is then

$$q(z) = N_D(z) + \sum_i \int_{\phi} \rho(E) |\chi f_i(E, z)|^2 dE, \quad (7.19)$$

where again the integral is over the set ϕ of all populated states, the summation is over all heterostructure subbands i , $f_i(z, E)$ is the multi-component envelope function for subband i at energy E , and χ is a diagonal matrix which selects only the populated components of the envelope function. The explicit form of χ is simple: for populated electron bands, $\chi_{ij} = 1$ if

basis state j is s -type, and 0 otherwise. For populated hole bands, $\chi_{ji} = 0$ if basis state j is s -type, and 1 otherwise. $N_D(z)$ is the charge density due to donors or interface charges (interface charges introduce a delta function spike in $N_D(z)$).

Eq. (7.19) is the proper expression for the charge density, but it is inconvenient to integrate over energy. Instead a substitution of variables is made to integrate over $k_{\parallel}$:

$$q(z) = N_D(z) + \sum_i \frac{1}{(2\pi)^2} \int_{\phi} |\chi_{ji}(k_{\parallel}, z)|^2 2\pi k_{\parallel} dk_{\parallel}. \quad (7.20)$$

In single-band models, the set of populated states ϕ is simply all $k_{\parallel} < k_F$, where k_F is the Fermi wave vector. In intrinsic structures, k_F is set as the point in $k_{\parallel}$ -space where the electron and hole bands uncross. In multi-band models, however, the concept of a Fermi wave vector is misleading, as bands far from the Γ point will still contain mixing terms, leading to slightly populated bands with $k_{\parallel} > k_F$, even at zero temperature. However, the majority of occupied states do occur for $k_{\parallel} < k_F$, and I find that the total carrier density of a structure is insensitive to whether the integration of Eq. (7.20) or Eq. (7.17) is carried out to $2k_F$ or $3k_F$.

Eq. (7.20) is the final expression for the charge distribution, and is explicitly solved in self-consistent multi-band models. For the purposes of integration (Eq. (7.18)) the energy bands are broken into discrete steps in $k_{\parallel}$ -space, contributions from which are then summed to provide both the total number of carriers in the structure and also the charge distribution.

Knowing the electronic structure of the heterostructure, Eqs. (7.18) and (7.20) allow one to calculate the electrostatic potential $V_{es}(z)$, and so the total band-edge potential $V(z)$.

7.3.1.5 Step 5: Determining convergence

Given the algorithm for self-consistent calculations presented above, it would seem a simple matter of solving the Schrödinger wave equation (SWE) and Poisson's equation several times until convergence was obtained. In practice, however, there are ways to improve the speed of convergence.

The most important point (from a convergence perspective) is how to incorporate a newly-calculated band-edge potential $V(z)$. If after each iteration, one simply replaces the old potential with the new, oscillations in carrier densities result that can ruin convergence. Instead, it is best to take a weighted average of the old and new potentials. For these

computationally-intensive calculations, I have found it best to write an algorithm which adjusts the weightings based on convergence of the carrier densities. If the densities between successive iterations change very little, then more of the new potential is included each iteration. If the carrier densities appear to be oscillating, then less of the new potential is added. This adjustable convergence parameter speeds convergence, and prevents oscillations in carrier density between iterations. Also, it mitigates the effect of my initial flatband guess at $V(z)$.

I find that 8 to at most 14 iterations are needed for convergence of energies and densities to better than 0.01 meV and 10^8 cm^{-2} , respectively. Even with few iterations, the energy bands must be calculated at a large number of $k_{\parallel}$ and q points for high accuracy. In addition, thick layers require more Fourier terms to be included in the momentum-matrix than thin layers, all of which increase execution time. Literally days of DEC Alpha CPU time can be required for the thickest layer structures presented here, although most structures were solved in a few hours on a desktop PC.

7.3.2 Simplifications used in the calculations

I make two important simplifications when performing these self-consistent calculations. To begin, I use the axial approximation, where the dispersion of the energy levels in the layer planes is assumed to be isotropic. This considerably simplifies the Hamiltonians involved, and reduces the complexity of self-consistent calculations by an order of magnitude. The second simplification is that I assume the majority of populated states occur at k_z extrema ($k_z = 0$ or π/d). Both of these simplifications therefore induce some quantitative error into the calculations, as the InAs/(Ga,In)Sb system is known to be anisotropic, and in some cases bands may have significant population at intermediate k_z values. However, as in the absorption case, the qualitative results presented here will not be affected by anisotropy or slight population redistribution.

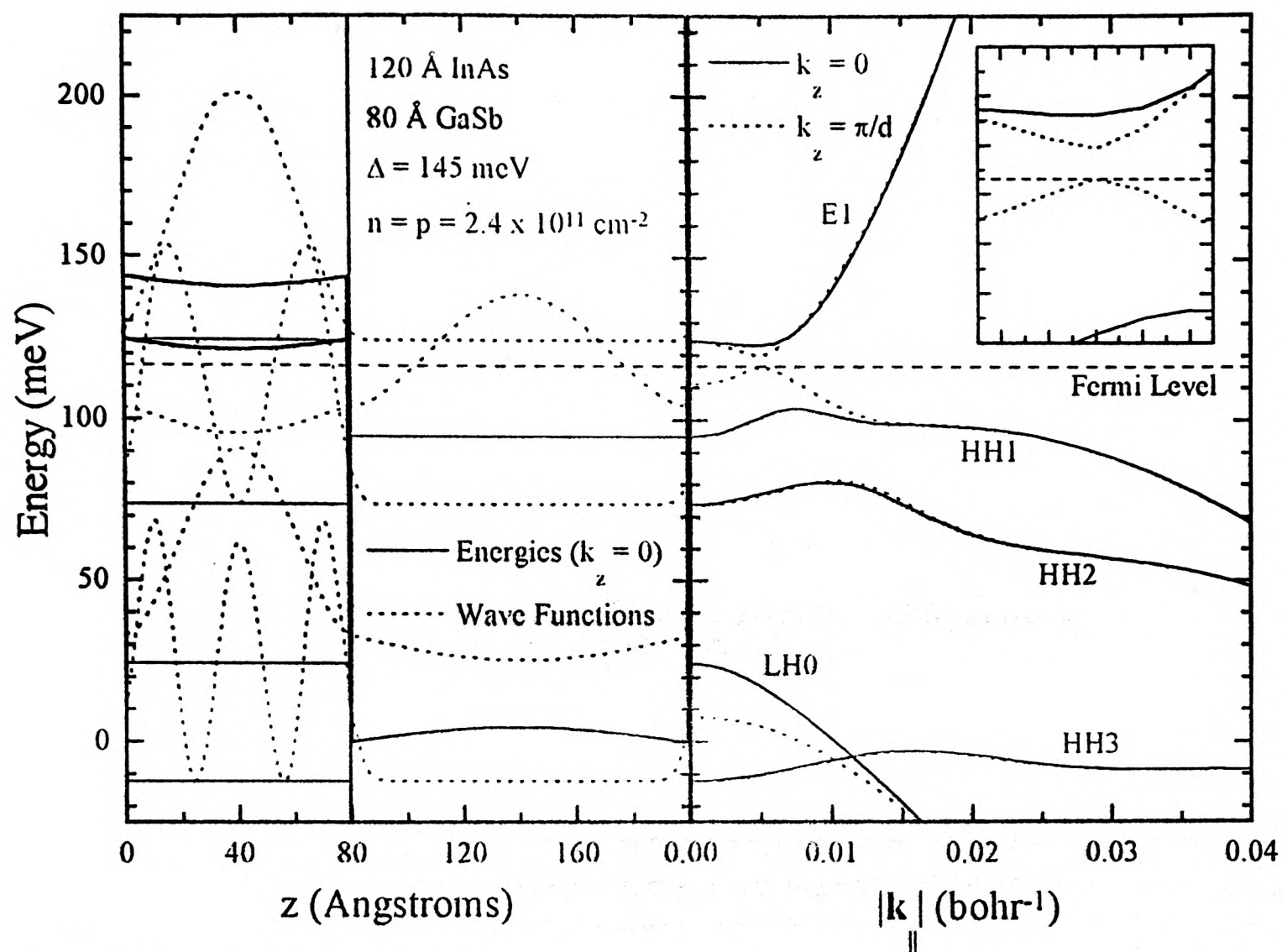


Figure 7.11: A composite picture of a semimetallic InAs/GaSb superlattice, layer widths as indicated. On the left are the Γ point wave functions and the band-edges (the valence band of GaSb has been split by compression, so the heavy hole edge has been raised). On the right is the $k_{||}$ -dispersion of the energy bands. This sample has a direct gap of ~ 3 meV (see inset).

7.3.3 "Band Gaps"

The results for three semimetallic superlattices are presented in Figs. 7.11-7.13. In Fig. 7.11 I plot a sample whose period is composed of a 120 Å InAs layer, and an 80 Å GaSb layer. These are the same thicknesses Altarelli uses in his example, and so Fig. 7.11 allows for a comparison with Altarelli's results. We are in excellent agreement for this sample, although we are using different band parameters, a slightly different band overlap (he uses 150 meV, I use 145 meV), different Hamiltonians, and different techniques. He finds a direct gap of 2 meV at the point $k_z = \pi/d$, $k_{||} = 0.43 \pi/d$, and I find a direct gap of 3.3 meV at the point $k_z = \pi/d$, $k_{||} = 0.60 \pi/d$. The valence band dispersions are slightly different for lower-lying bands, but this is probably due to Altarelli's use of the spherical approximation, and different γ parameters.

In Fig. 7.12, an InAs/GaSb superlattice with layer thicknesses of 220 Å InAs and 120 Å GaSb has been calculated, assuming intrinsic electron and hole populations. These parameters are similar to sample 1249 [001], which is determined from transport

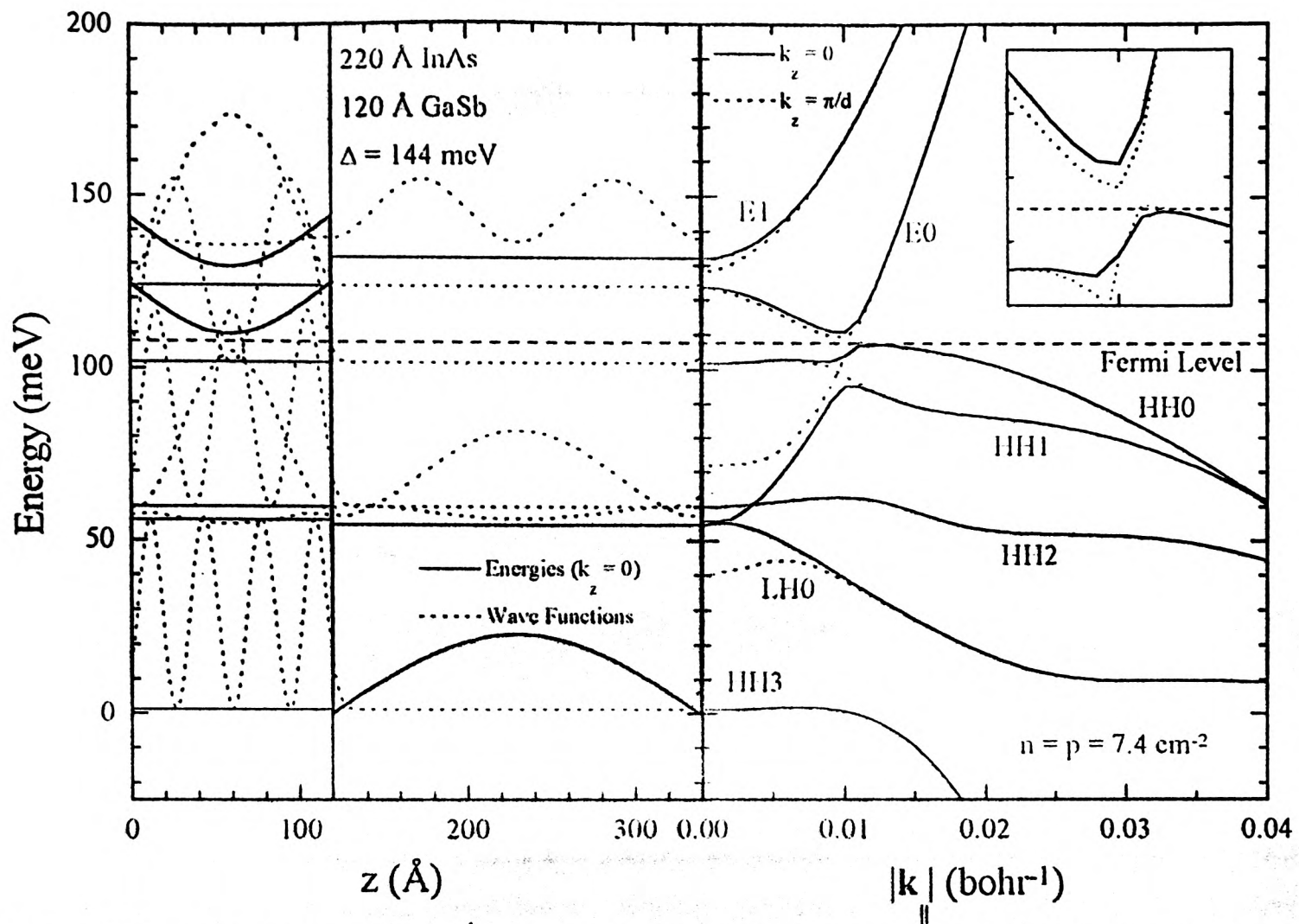


Figure 7.12: A composite picture of a semimetallic InAs/GaSb superlattice, layer widths as indicated. On the left are the Γ point wave functions and the band-edge. On the right is the k_z -dispersion of the energy bands. This sample has a small indirect gap, although a Fermi surface does exist (see inset).

measurements to have a carrier density of $\sim 6.5 \times 10^{11} \text{ cm}^{-2}$. The calculated carrier density of $7.4 \times 10^{11} \text{ cm}^{-2}$ indicates that the band overlap of 144 meV fitted in the effective-mass approximation may be too large. Transport measurements indicate that only one electron and hole state are populated in a superlattice period, and the band structure agrees with that.

For these thicknesses, Altarelli's claim of zero or small band gap semiconductors no longer holds. From the inset of Fig. 7.12, it is seen that although a small indirect band gap exists, there is a well-defined Fermi surface (the energy bands at $k_z = \pi/d$ pierce the Fermi level). Altarelli found that for thin-layer superlattices, semimetallic behavior could only be explained by extrinsic effects. For thick-layer superlattices, it is clear that the bands exhibit semimetallic behavior in a completely intrinsic environment.

A superlattice with even thicker layers is presented in Fig. 7.13. These layer thicknesses have been chosen to match 1546 [001], which had electron and hole populations of 7.2 and $4.6 \times 10^{11} \text{ cm}^{-2}$, respectively. Interface charge was added to account for the imbalance, but the calculation predicts larger carrier densities, indicating that a band overlap of 140 meV is probably too large. Even with this larger band overlap, only two conduction states are found to be populated. Single band models have consistently predicted three

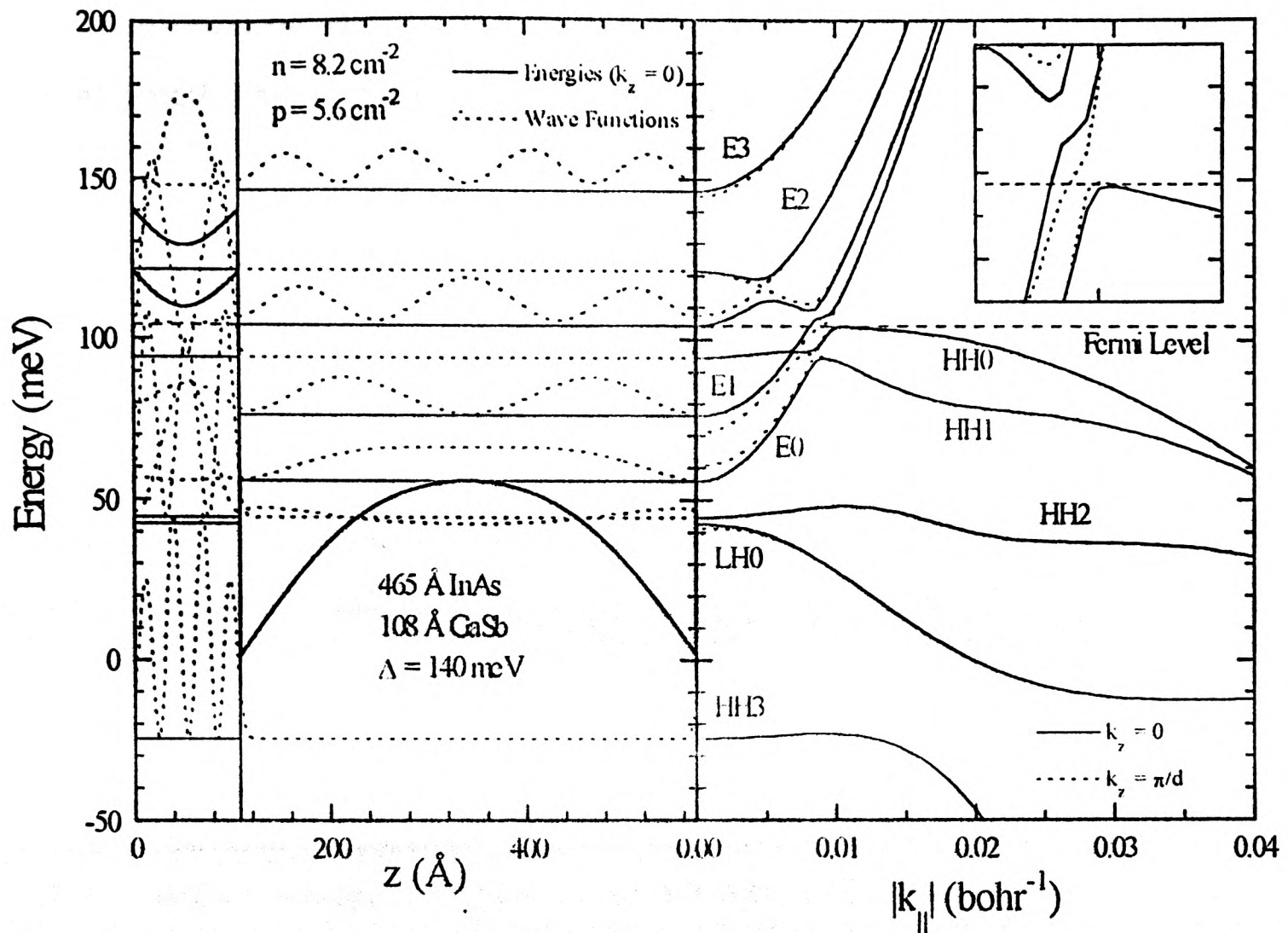


Figure 7.13: A composite picture of a semimetallic InAs/GaSb superlattice, layer widths as indicated. On the left are the Γ point wave functions and the band-edges (the valence band of GaSb has been split by compression, so the heavy hole edge has been raised). On the right is the $k_{||}$ -dispersion of the energy bands. This sample has no band gap, and both electron and hole bands cut through the Fermi level (see inset).

populated conduction states in superlattices with InAs widths over 400 Å [35]. This multi-band calculation agrees with transport measurements [20], which find only two conduction states populated. For all samples modeled, in both single- and multi-band formulations, only one heavy hole state is found to be populated.

Quinn and Quinn [36] use a simple coupled model (with no self-consistency) and the results of Altarelli [5] to conclude that for intrinsic superlattices, the Fermi level is always in the band gap of the system, and that a band gap always exists until the layers are wide enough for a second electron state to become populated, at which point a Fermi surface exists. However, the results here indicate that there is in fact no hard rule about wide-layer superlattices with only one populated electron level. Although such structures are expected to have a gap of some sort, a Fermi surface may well exist. This is most likely because of the strong band mixing, where light hole states below the Fermi surface will contain strong electron-like character, leading to a large electron population that can only be compensated for by a low Fermi level, often low enough to fall out of the gap and result in a Fermi surface.

7.3.4 Far-Infrared Interband Detectors

Although the self-consistent procedure takes considerably more computer time than a simple semiconducting calculation, the end result is the same: energy bands and wave functions for the heterostructure, and the Fermi level. Therefore, once the bands have been calculated, absorption in a semimetallic structure can be calculated in the same manner as in the semiconducting case. Here I

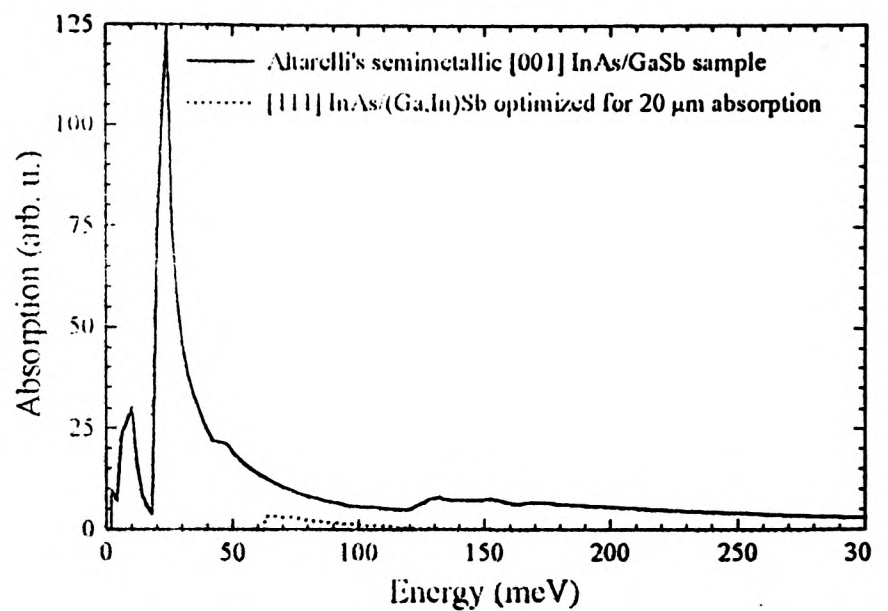


Figure 7.14: The absorption of a semimetallic structure (see Fig. 7.11), compared to an optimized semiconducting structure.

define “semimetallic” loosely, as any structure in which charge transfer has taken place ($E_0 < HH_0$), irrespective of whether a Fermi surface exists. In fact, it will be shown that optimum detectors are exactly those structures in which charge transfer has taken place, but no Fermi surface exists.

The results for an absorption calculation are shown in Fig. 7.14 (calculated from the bands in Fig. 7.11). Absorption below 20 meV is due to $E_0 \rightarrow HH_0$ transitions at $k_z = \pi/d$, forbidden at $k_{||} = 0$ but allowed for general $k_{||}$. The absorption is orders of magnitude larger than for a semiconducting sample. This strong absorption is due to the band gap appearing at a finite $k_{||}$ value. As is clear from Eq. (7.14), if the JDOS has a strong maximum (bands parallel) at $k_{||} \approx 0$, the total absorption will still be small. However, if the JDOS is large for finite $k_{||}$ (as is usually the case for semimetallic structures), then the absorption will be much larger.

In practice, of course, metals are not very good detectors, since ideally one hopes for large changes in resistance when absorption occurs. However, by properly engineering the structure, semimetallic InAs/(Ga,In)Sb superlattices may be designed such that charge transfer occurs with a large JDOS at finite $k_{||}$, with the Fermi level situated in the middle of a band gap (no Fermi surface).

Calculated absorption in several semimetallic superlattices is presented in Fig. 7.15. The absorption is several orders of magnitude larger than the semiconducting superlattice optimized in Fig. 7.9 (a semiconducting superlattice optimized to absorb at 40 meV would

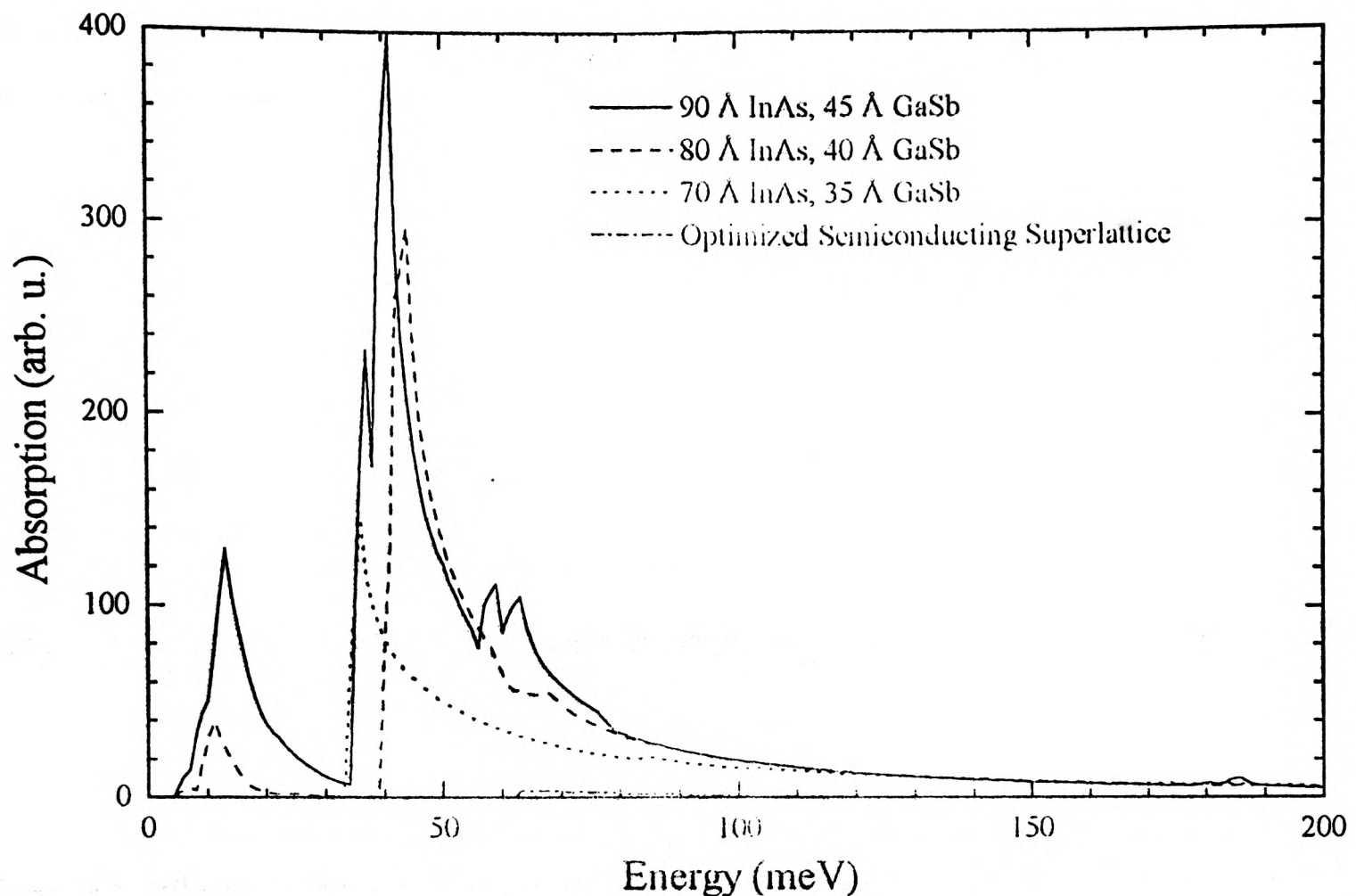


Figure 7.15: Absorption of semimetallic [111] InAs/(Ga,In)Sb superlattices, compared to the optimized 20 μm semiconducting superlattice of Fig. 7.9. Note that in all cases, a band gap exists.

have even weaker absorption). As in the semiconducting case, [111] superlattices with indium incorporated into the GaSb layers are preferred. In this case, the thinner layers lead to stronger band coupling, such that sizable band gaps open up in these semimetallic structures (of order 10 meV). The absorption below the 40 meV peak is due to absorption at $k_z = \pi/d$. The layer width dependence of the peak absorption is complex. In general, for a given desired absorption energy, increasing the layer widths will increase the absorption strength (due to large regions of parallel bands), at the cost of shrinking the band gap. A band gap of several meV is desired, such that thermal excitation will not swamp absorption. These preliminary results indicate that strong high-temperature ($k_B T \sim 10$ meV, or $T \sim 100$ K) absorption of 20-40 μm radiation is possible, using these wide layer [111] InAs/(Ga,In)Sb superlattices.

7.4 Magnetic Fields in Intrinsic Systems

The problem of magnetic fields in intrinsic, multi-band systems has not been investigated at all, as far as I am aware. In principle, the self-consistent algorithm presented earlier can be used with systems with an applied field, but the extra degree of quantization provided by the field makes the calculation somewhat more difficult. In particular, the carrier concentration is extremely sensitive to the exact Fermi and Landau level energies. In the zero

field case, the k -space dispersion of the energy bands means that a small error in the Fermi level will lead to only a minor discrepancy in carrier density. With an applied field, a slight error in either the Fermi level or a Landau level will result in the population or depopulation of an entire Landau state, which for high fields ($B > 1$ T) can have drastic consequences on the carrier density. Also, intrinsic systems have as a consequence of charge balance the fact that electron and hole states must cross the Fermi level at the same time. However, the intrinsic numerical error of computers (even if only 1 part in 10^{16}) means that no two bands will ever have the *exact* same energy. The solution is to incorporate temperature effects, such that bands will be somewhat populated if they are within $k_B T$ of the Fermi level. This temperature-induced broadening makes self-consistent calculations of intrinsic systems in magnetic fields possible.

7.4.1 Simple Model

Although I present results for the full 8-band case, it is useful to see the qualitative results of a simple, decoupled model. These results are used to explain the curious oscillations in cyclotron resonance (CR) linewidth and intensity observed in Chapter 3.

Only one electron and one hole state are assumed to be populated, and their energies are written as explicit functions of the carrier density and magnetic field:

$$\begin{aligned} E_{ei}(B, n) &= \alpha n + (i + 1/2) \frac{B}{m_e^*}, \\ E_{hj}(B, n) &= \Delta - \beta n - (j + 1/2) \frac{B}{m_h^*}, \end{aligned} \quad (7.21)$$

where n is the carrier density ($n = p$), B is the magnetic field, m_e^* and m_h^* are the carrier effective masses, and E_{ei} and E_{hj} are the i^{th} electron and j^{th} hole Landau levels, respectively. Δ is the separation between the zero-field electron and hole levels, with no self-consistency (so in practice Δ is somewhat less than the band overlap). The coefficients α and β parameterize the effects of the self-consistent Coulomb potential (here I assume that the potential shifts the energies linearly with carrier density, although any explicit function may be used). I use the values $m_e^* = 0.025$, $m_h^* = 0.25$, $\alpha = 8 \times 10^{-11}$ meV cm², $\beta = 6 \times 10^{-11}$ meV cm², and $\Delta = 140$ meV. The masses and Δ value are close to those observed in multi-band calculations,

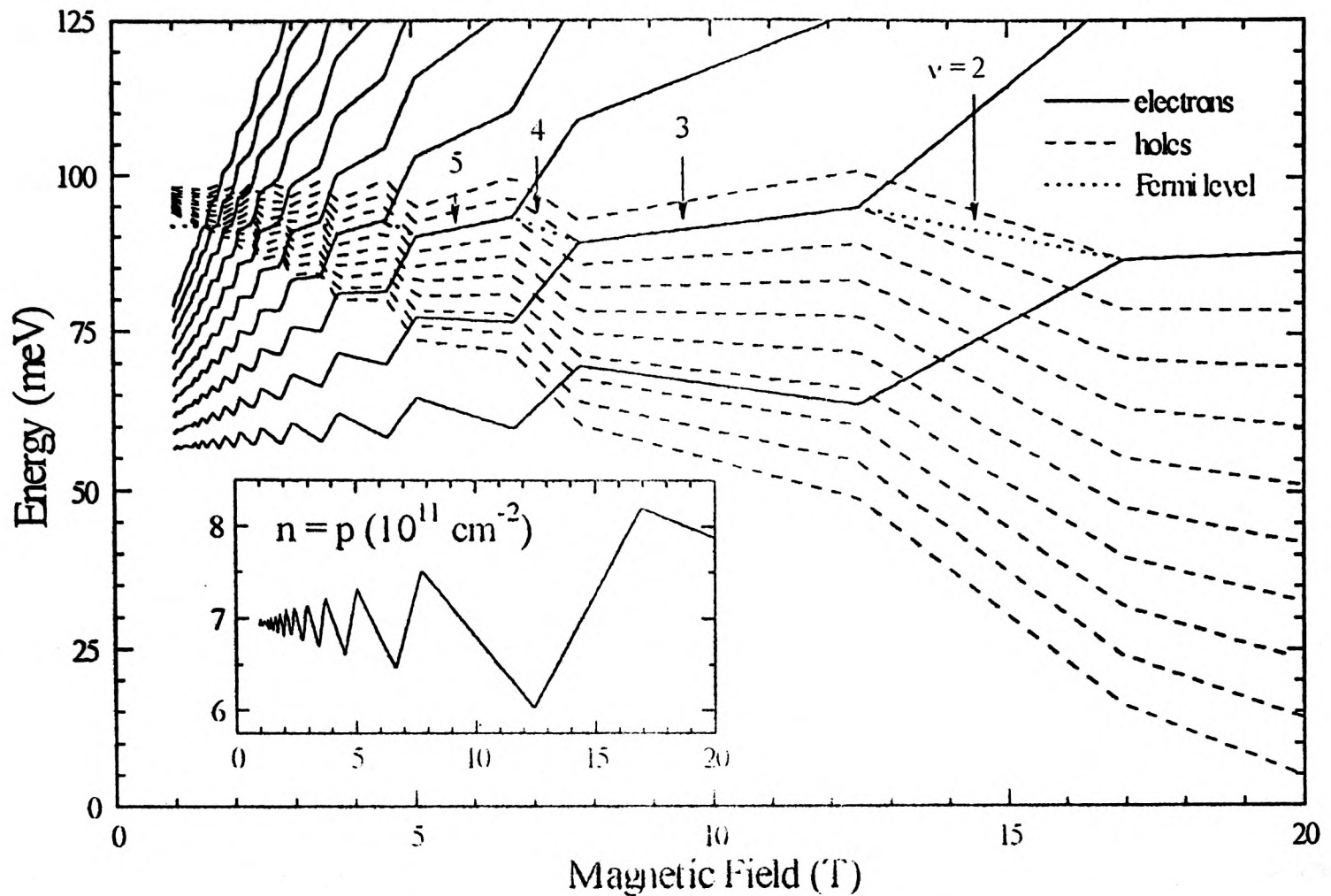


Figure 7.16: Results of the simple intrinsic model in magnetic field, for the first 10 Landau levels. Filling factors are labeled assuming a constant carrier density of $6.95 \times 10^{11} \text{ cm}^{-2}$ (the actual field-dependent carrier density is inset). In general, even filling factors occur when the Fermi level is between (spin-degenerate) Landau levels, and odd filling factors occur when the Fermi level, electron state, and hole state are “pinned” together.

and α and β are likewise based on calculated energy level shifts with carrier density, but I am more concerned with qualitative behavior than precise results.

The only differences between Eq. (7.21) and standard effective-mass magnetic field equations are the carrier-density-dependent terms proportional to α and β , and it is through them that intrinsic self-consistency is obtained. For a given magnetic field value B , the carrier density n is tuned (via an iterative procedure) to the unique value n such that equal numbers of electron and hole states are populated, *i.e.* $n = p$. This simple model is quick to implement, and requires no broadening for the self-consistent iterations to work.

The calculated Landau level fan is shown in Fig. 7.16. An odd oscillatory structure appears in the Landau levels, a result of the carrier density oscillating. There are two regimes of behavior. When the Fermi level is between levels, the density increases, and so the band-bending pushes the bound states further out of their respective wells. When the Fermi level is pinned to the highest populated electron and hole states, the states depopulate with field, which relaxes the Coulombic potential. These oscillations, and their dependence on filling

factor, were used in Chapter 3 to explain the curious oscillations seen in heterojunction CR (for the model in Chapter 3, nonparabolicity of the conduction band was included as well).

The simple model therefore exhibits striking qualitative behavior, which has already helped to explain some hitherto unexplained experimental results. However, although some oscillations are seen in CR, wild variations in carrier density are not in general observed with magnetic field. In addition, the bound states of an InAs/(Ga,In)Sb heterojunction will include strong electron-hole mixing, which is expected to affect the energies somewhat. For a quantitative description to better compare with experimental results, I turn back to the multi-band momentum-matrix formulation.

7.4.2 Multi-Band Treatment

The same basic self-consistent algorithm is used for magnetic field systems as was used for zero-field systems. The Hamiltonian used to calculate the eigenstates will be different, where the momentum operators in the plane k_x, k_y are replaced by ladder operators $a^\dagger, a$ (see Chapter 2 and Table A.5 in the Appendix). Instead of subbands with a k_x -dispersion, the bound states of the systems will be Landau levels.

As was mentioned earlier, the complete quantization of the system due to the magnetic field makes a self-consistent treatment difficult. Therefore, temperature broadening is included to “smooth” out the Landau levels. The form of broadening is simply the Fermi filling function

$$f(E) = \frac{1}{1 + \exp[(E - E_F) / k_B T]} \quad (7.22)$$

where E_F is the Fermi level of the structure. The electron population of a given Landau level n_i of energy E is then

$$n_i(E) = f(E) n_D \quad (7.23)$$

where n_D is the degeneracy of a non-spin-degenerate Landau level

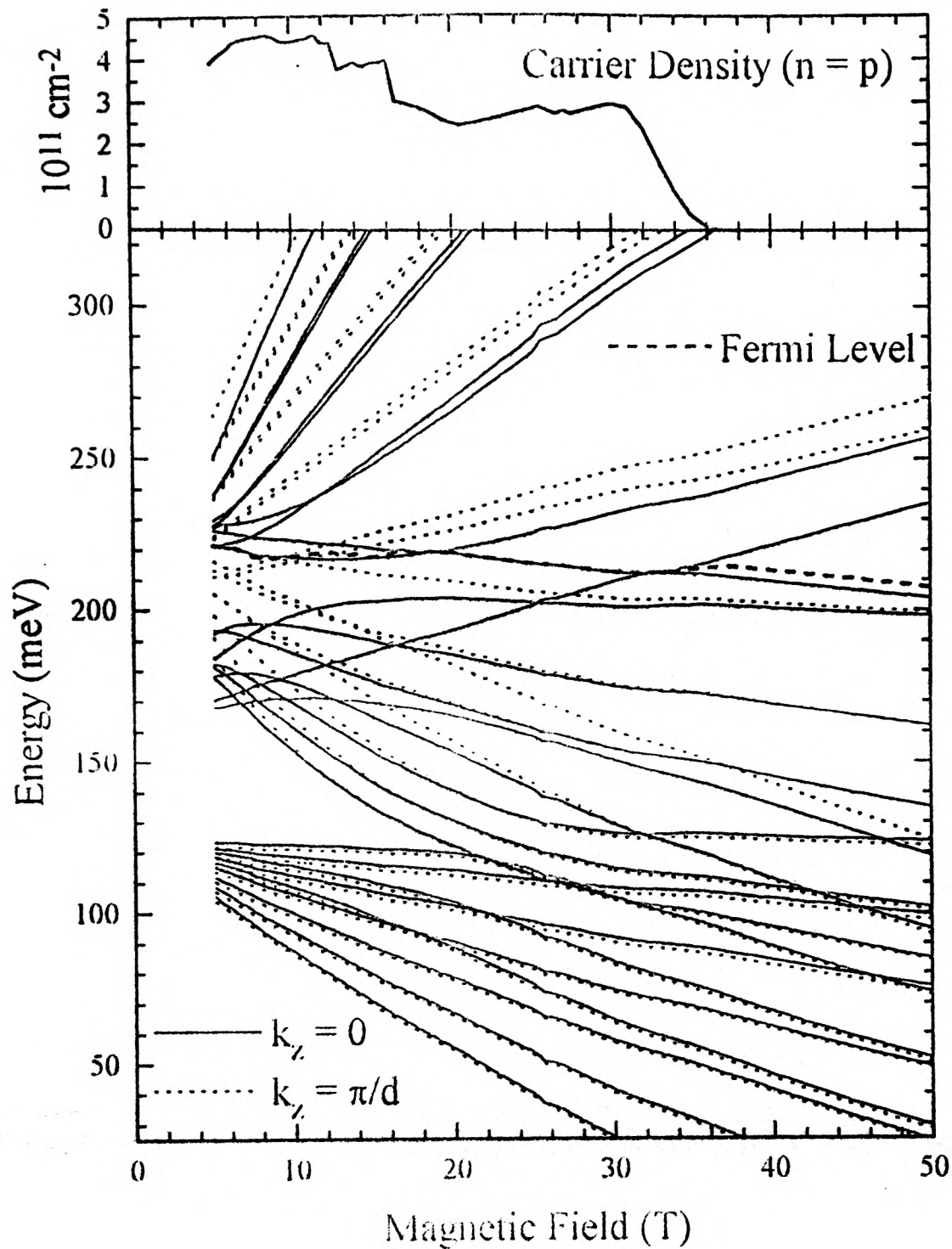


Figure 7.17: Self-consistent calculation of a [111] 90 Å InAs/36 Å (Ga,In)Sb superlattice (15% indium).

$$n_D = \frac{B}{2\pi}. \quad (7.24)$$

In a multi-band formalism, the electron population calculated from Eq. (7.23) will be further modulated by the amount of electron mixing in the Landau level.

The self-consistent algorithm proceeds as before. Given a potential, the magnetic-field Hamiltonian is used to find the bound states of the system. The Fermi level is calculated, again with an iterative procedure, using the broadening of the Landau levels to determine an energy such that charge balance is satisfied. No k -space integration is required to calculate the charge distribution $q(z)$. Instead, the population of each state is modulated by its envelope function. The calculation of the Coulomb potential is therefore faster for the magnetic field

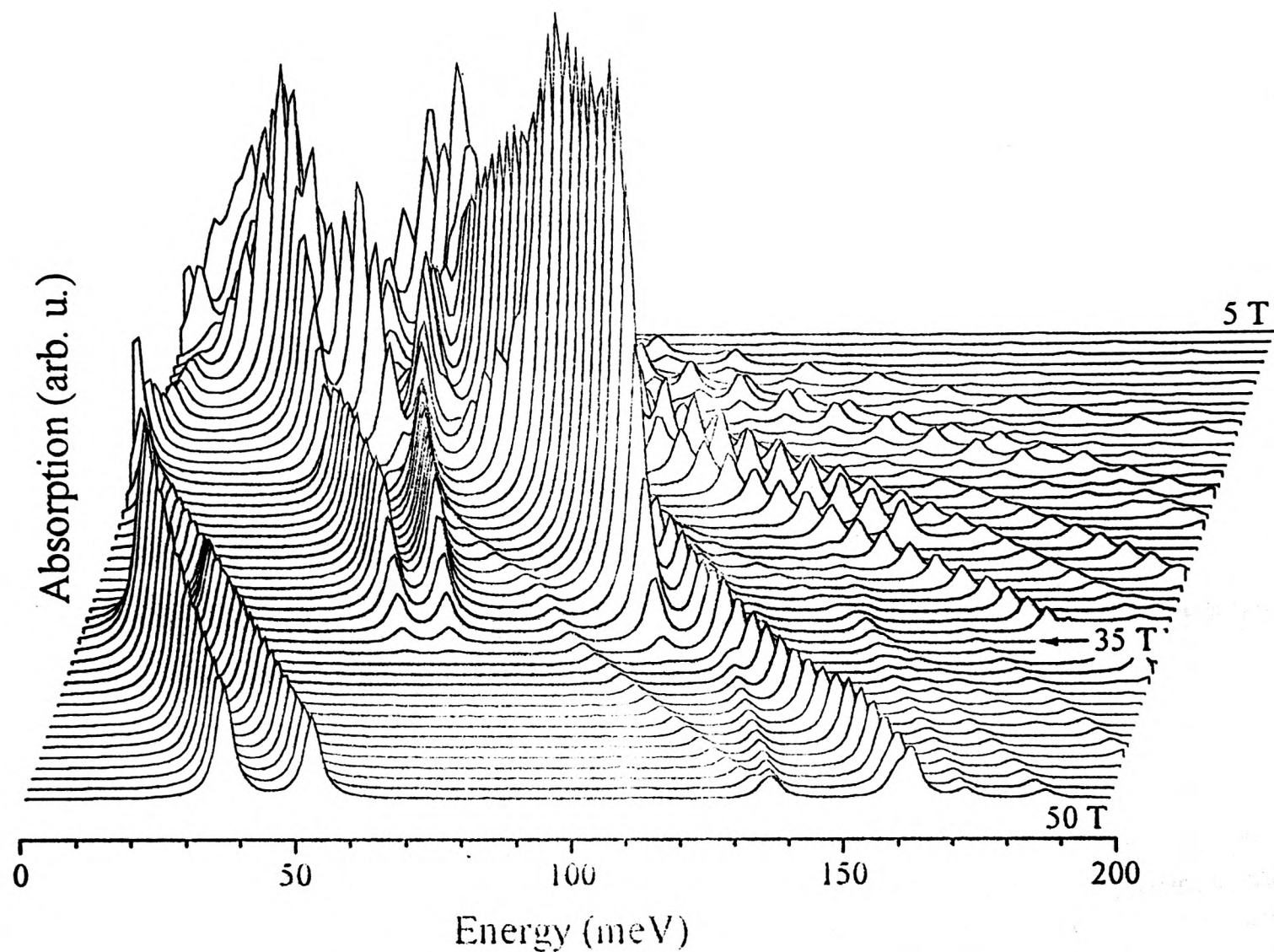


Figure 7.18: Complicated mixture of CR and interband transitions calculated from the band structure of Fig. 7.17. Note the disappearance of CR transitions as the superlattice becomes semiconducting at ~ 35 T.

case than the zero-field case. The overall calculation takes longer, however, because a full 8×8 Hamiltonian must be used, rather than separate 4×4 's.

A sample calculation is presented in Fig. 7.17. Although oscillations in carrier density still occur, and so give rise to slight oscillations in the Landau levels of the system, the oscillations are smoother than for the simple model of Fig. 7.16. This damping of the oscillations is due to band mixing and broadening. Again, electron and hole levels cross the Fermi level together (19 and 35 T). In this case, the superlattice becomes semiconducting at a field of 35 T. Thicker superlattices exhibit the same qualitative results: regions of populating and depopulating Landau levels, leading to oscillations in carrier density and Landau structure.

From these results, and the oscillations in mass, linewidth and intensity observed in InAs/GaSb heterojunctions presented in Chapter 3, it is clear that intrinsic systems behave very differently from extrinsic systems such as GaAs/AlGaAs.

7.4.3 Magnetic Field Transitions

From the selection rules presented in Chapter 2, the absorption of intrinsic structures can be calculated once the Landau levels are known. The absorption spectrum as calculated from magnetic field selection rules is a series of delta functions of varying strength, here Lorentzian broadening is used to simulate broadening observed in experiment.

The calculated transitions for the sample presented in Fig. 7.17 are shown in Fig. 7.18, with a constant broadening full-width at half-maximum $\Gamma = 3.5$ meV. Due to the thin layers involved (90 Å InAs, 36 Å InGaSb), both interband and cyclotron transitions are strong. The electron cyclotron resonance ($m^* = 0.035 m_0$) dominates until the superlattice becomes semiconducting, after which several interband transitions are visible. For this thin layer superlattice the hole mass has been reduced (the two hole transitions have masses $m^* = 0.067$ and $0.058 m_0$), as has been observed by Onaggio *et al.* [37] in [001] superlattices with large indium content.

7.5 Conclusions

In this chapter the EFA has been used, via the momentum-matrix technique, to calculate the electronic structure and absorption spectra of InAs/(Ga,In)Sb superlattices. Semiconducting superlattices are shown to exhibit optimum optical response when the InAs layers are thick relative to the (Ga,In)Sb barrier layers. Semimetallic superlattices are calculated via a self-consistent algorithm, and are predicted to absorb strongly at far-infrared wavelengths. Finally, intrinsic multi-band systems in magnetic fields are investigated for the first time, showing oscillations in carrier density and energy levels.

7.6 References

- [1] G. A. Sai-Halasz, R. Tsu, and L. Esaki, Appl. Phys. Lett. **30** (1977) 651.
- [2] L. L. Chang, N. Kawai, G. A. Sai-Halasz, R. Ludeke, and L. Esaki, Appl. Phys. Lett. **35** (1979) 939.
- [3] L. L. Chang, J. Phys. Soc. Japan **49** (1980) A 997.
- [4] G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **26** (1982) 1974.
- [5] M. Altarelli, Phys. Rev. B **28** (1983) 512.
- [6] P. Voisin, G. Bastard, and M. Voos, Phys. Rev. B **29** (1984) 935.
- [7] D. L. Smith and C. Mailhot, J. Appl. Phys. **62** (1987) 2545.

- [8] C. H. Grein, H. Cruz, M. E. Flatte, and H. Ehrenreich, *Appl. Phys. Lett.* **65** (1994) 2530.
- [9] J. H. Roslund and T. G. Andersson, *Super. Micro.* **16** (1995) 77.
- [10] E. R. Heller, K. Fisher, F. Szmulowicz, and F. L. Madarasz, *J. Appl. Phys.* **77** (1995) 5739.
- [11] J. P. Loehr, *Appl. Phys. Lett.* **67** (1995) 2509.
- [12] C. H. Grein, P. M. Young, and H. Ehrenreich, *J. Appl. Phys.* **76** (1994) 1940.
- [13] M. P. Houn, Y. H. Wang, H. H. Chen, and Y.-C. Chang, *Super. and Micro.* **13** (1993) 181.
- [14] R. J. Warburton, *D. Phil Thesis*, Clarendon (1991).
- [15] G. E. Pikus and G. L. Bir, *Sov. Phys. Solid State* **1** (1960) 1502.
- [16] C. G. Van de Walle, *Phys. Rev. B* **39** (1989) 1871.
- [17] J. Los, A. Fasolino, and A. Catellani, to be published in *Phys. Rev. B* (1996).
- [18] C. G. Van de Walle and R. M. Martin, *Phys. Rev. B* **34** (1986) 5621.
- [19] D. L. Smith, *Solid State Comm.* **57** (1986) 919.
- [20] D. M. Symons, *D. Phil Thesis*, Clarendon (1994).
- [21] J. R. Waterman, B. V. Shanabrook, R. J. Wagner, M. J. Wagner, M. J. Yang, J. L. Davis, and J. P. Omaggio, *Semicond. Sci. Tech.* **8** (1993) S106.
- [22] D. M. Symons, M. Lakrimi, R. J. Warburton, R. J. Nicholas, N. J. Mason, P. J. Walker, M. I. Eremets, and G. Hill, *Phys. Rev. B* **49** (1994) 16614.
- [23] D. M. Symons, M. Lakrimi, R. J. Warburton, R. J. Nicholas, N. J. Mason, P. J. Walker, and M. I. Eremets, *Semicond. Sci. Tech.* **9** (1994) 118.
- [24] D. M. Symons, M. Lakrimi, M. van der Burgt, T. A. Vaughan, R. J. Nicholas, N. J. Mason, and P. J. Walker, *Phys. Rev. B* **51** (1995) 1729.
- [25] J. R. Meyer, C. A. Hoffman, B. V. Shanabrook, B. R. Bennett, R. J. Wagner, J. R. Waterman, and E. R. Youngdale, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, World Scientific, Singapore, 1995, pg. 783.
- [26] J. M. Luttinger and W. Kohn, *Phys. Rev.* **97** (1955) 869.
- [27] M. G. Burt, *J. Phys. Cond. Matt.* **4** (1992) 6651.
- [28] M. W. Wang, D. A. Collins, T. C. McGill, R. W. Grant, and R. M. Feenstra, *Appl. Phys. Lett.* **66** (1995) 2981.

- [29] See the growth references in Chapter 1.
- [30] T. A. Vaughan, M. Lakrimi, R. J. Nicholas, N. J. Mason, and P. J. Walker, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, World Scientific, Singapore, 1995, pg. 1256.
- [31] A. M. Cohen, G. E. Marques, Phys. Rev. B 41 (1990) 10608.
- [32] C. Kittel, *Quantum Theory of Solids*, John Wiley & Sons, New York, 1963, Chapter 5: "Fermion Fields and the Hartree-Fock Approximation."
- [33] F. Szmulowicz, M. O. Manasreh, C. E. Stutz, and T. Vaughan, Phys. Rev. B 50 (1994) 11618.
- [34] W. L. Bloss, J. Appl. Phys. 66 (1989) 3639.
- [35] D. Symons, private communication.
- [36] J. J. Quinn and J. J. Quinn, in *Proceedings of the 11th Conference on the Electronic Properties of Two-Dimensional Systems*, Nottingham, August 7-11 1995.
- [37] J. P. Omaggio, J. R. Meyer, R. J. Wagner, C. A. Hoffman, M. J. Yang, D. H. Chow and R. H. Miles, Appl. Phys. Lett. 61 (1992) 207.

Chapter 8

Conclusions

This thesis has studied the optical properties of InAs/GaSb heterostructures under applied magnetic fields. The unusual crossed-gap nature of the InAs/GaSb band lineups allows for the design of thin layer structures with far-infrared band gaps, and provides a high density of intrinsic carriers for thick layer structures.

The cyclotron resonance studies of the system are useful characterization, providing information about the variation of carrier effective masses on growth orientation and layer widths. Cyclotron resonance of heterojunctions reveals oscillations in effective mass, linewidth and intensity that are unique to intrinsic systems. Studies at high intensity show evidence of the magnetophonon effect, and allow for a direct measurement of the LO-phonon-assisted energy relaxation rate. Coupled cyclotron resonance provides information about the subband separation energies, and the coupling matrix elements between subbands.

Optical studies of thin-layer systems show the promise of InAs/GaSb in far-infrared device applications. The band gaps of InAs/GaSb superlattices are shown to be easily tunable through a wide range of far-infrared energies, and vertical transport results indicate that this system will function reliably in a device environment.

The theory presented in this thesis centered on the envelope function approximation, an extension of $k \cdot p$ theory to heterostructures. The theory has proved to be remarkably successful in analyzing experimental results, and has predicted ways of improving the performance of the system. In addition, the effects of magnetic fields on intrinsic systems were studied quantitatively for the first time.

The end result of experimental and theoretical investigation shows the InAs/GaSb to be a relatively mature system, in the sense that many observed properties can now be predicted and explained by theory. The high quality of the samples studied also attests to the maturity of the growth technology. However, in almost every case it is seen that the unique characteristics of the InAs/GaSb have yet to be fully exploited, and the unusual quantum and intrinsic features of this system will very likely engage theorists and experimentalists even after commercial devices are developed.

Appendix A

k·p Matrices

Table A.1: The block-diagonalized bulk Hamiltonian (zero-field only, see Chapter 2) for [001] and [111] orientations. The upper triangle is the Hermitian conjugate of the lower triangle.

	<i>c</i>	<i>hh</i>	<i>lh</i>	<i>so</i>
<i>c</i>	$(F + \frac{1}{2}) k^2 + E_G$			$k_{\parallel} = (k_x, k_y)$
<i>hh</i>	$\sqrt{\frac{1}{2}} P k_{\parallel} $	$-\frac{1}{2} (\gamma_1 - 2 \gamma_x) k_z^2$ $-\frac{1}{2} (\gamma_1 + \gamma_x) k_{\parallel}^2$		
<i>lh</i>	$\frac{1}{\sqrt{6}} P k_{\parallel} $ $-i \sqrt{\frac{2}{3}} P k_z$	$-\frac{\sqrt{3}}{2} \beta k_{\parallel}^2$ $+ i \sqrt{3} \alpha k_{\parallel} k_z$	$-\frac{1}{2} (\gamma_1 + 2 \gamma_x) k_z^2$ $-\frac{1}{2} (\gamma_1 - \gamma_x) k_{\parallel}^2$	
<i>so</i>	$\frac{1}{\sqrt{3}} P k_{\parallel} $ $+ \frac{i}{\sqrt{3}} P k_z$	$-\sqrt{\frac{3}{2}} \beta k_{\parallel}^2$ $-i \sqrt{\frac{3}{2}} \alpha k_{\parallel} k_z$	$\sqrt{2} \gamma_x k_z^2 - \sqrt{\frac{1}{2}} \gamma_x k_{\parallel}^2$ $-i \frac{3}{\sqrt{2}} \alpha k_{\parallel} k_z$	$-\frac{1}{2} \gamma_1 k^2 - \Delta$

Table A.2: Orientation-dependent parameters used in the Hamiltonians.

Parameter	[001]	[111]
γ_x	γ_2	γ_3
α	γ_3	$\frac{1}{3} (2 \gamma_2 + \gamma_3)$
β	$\frac{1}{2} (\gamma_2 + \gamma_3)$	$\frac{1}{3} (\gamma_2 + 2 \gamma_3)$

Table A.3: The 8-band zero-field bulk $k \cdot p$ Hamiltonian for the $[001]$ orientation. The upper triangle is the Hermitian conjugate of the lower triangle.

	$c \uparrow$	$lh \uparrow$	$lh \downarrow$	$so \downarrow$	$c \downarrow$	$hh \downarrow$	$lh \uparrow$	$so \uparrow$	
$ ^1/2, +^1/2\rangle$	$(F + \frac{1}{2})k^2 + E_G$								$c \uparrow$
$ ^3/2, +^3/2\rangle$	$\frac{1}{\sqrt{2}}P k_-$	$-\frac{1}{2}(\gamma_1 - 2\gamma_2)k_z^2$ $-\frac{1}{2}(\gamma_1 + \gamma_2)k_+ k_-$							$hh \uparrow$
$ ^3/2, -^1/2\rangle$	$\frac{1}{\sqrt{6}}P k_+$	$-\frac{\sqrt{3}}{2}(\mu k_-^2 + \beta k_+^2)$	$-\frac{1}{2}(\gamma_1 + 2\gamma_2)k_z^2$ $-\frac{1}{2}(\gamma_1 - \gamma_2)k_+ k_-$						$lh \downarrow$
$ ^1/2, -^1/2\rangle$	$\frac{1}{\sqrt{3}}P k_+$	$-\frac{\sqrt{3}}{2}(\mu k_-^2 + \beta k_+^2)$	$\frac{\sqrt{2}}{\sqrt{2}}\gamma_2 k_z^2$ $-\frac{1}{\sqrt{2}}\gamma_2 k_+ k_-$	$-\frac{1}{2}\gamma_1 k^2 - \Delta$					$so \downarrow$
$ ^1/2, -^1/2\rangle$	0	0	$-\frac{\sqrt{2}}{3}P k_z$	$\frac{1}{\sqrt{3}}P k_z$	$(F + \frac{1}{2})k^2 + E_G$				$c \downarrow$
$ ^3/2, -^3/2\rangle$	0	0	$\sqrt{3}\gamma_3 k_+ k_z$	$-\frac{\sqrt{3}}{2}\gamma_3 k_+ k_z$	$\frac{1}{\sqrt{2}}P k_+$	$-\frac{1}{2}(\gamma_1 - 2\gamma_2)k_z^2$ $-\frac{1}{2}(\gamma_1 + \gamma_2)k_+ k_-$			$hh \downarrow$
$ ^3/2, +^1/2\rangle$	$\frac{\sqrt{2}}{3}P k_z$	$-\sqrt{3}\gamma_3 k_+ k_z$	0	$-\frac{3}{\sqrt{2}}\gamma_3 k_+ k_z$	$\frac{1}{\sqrt{6}}P k_-$	$-\frac{\sqrt{3}}{2}(\beta k_-^2 + \mu k_+^2)$	$-\frac{1}{2}(\gamma_1 + 2\gamma_2)k_z^2$ $-\frac{1}{2}(\gamma_1 - \gamma_2)k_+ k_-$		$lh \uparrow$
$ ^1/2, +^1/2\rangle$	$-\frac{1}{\sqrt{3}}P k_z$	$\frac{\sqrt{3}}{2}\gamma_3 k_+ k_z$	$\frac{3}{\sqrt{2}}\gamma_3 k_- k_z$	0	$\frac{1}{\sqrt{3}}P k_-$	$-\frac{\sqrt{3}}{2}(\beta k_-^2 + \mu k_+^2)$	$\frac{\sqrt{2}}{\sqrt{2}}\gamma_2 k_z^2$ $-\frac{1}{\sqrt{2}}\gamma_2 k_+ k_-$	$-\frac{1}{2}\gamma_1 k^2 - \Delta$	$so \uparrow$
	$ ^1/2, +^1/2\rangle$	$ ^3/2, +^1/2\rangle$	$ ^3/2, -^1/2\rangle$	$ ^1/2, -^1/2\rangle$	$ ^1/2, -^1/2\rangle$	$ ^3/2, -^1/2\rangle$	$ ^3/2, +^1/2\rangle$	$ ^1/2, +^1/2\rangle$	

Table A.4: The 8-band zero-field bulk $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the $[111]$ orientation. The upper triangle is the Hermitian conjugate of the lower triangle.

	$c \uparrow$	$lh \uparrow$	$so \downarrow$	$c \downarrow$	$hh \downarrow$	$lh \uparrow$	$so \uparrow$
$ ^1/2, +^1/2\rangle$	$(F + \frac{1}{2})k^2 + E_G$						$c \uparrow$
$ ^3/2, +^3/2\rangle$	$\frac{1}{\sqrt{2}} P k_-$	$-\frac{1}{2}(\gamma_1 - 2\gamma_3)k_z^2$ $-\frac{1}{2}(\gamma_1 + \gamma_3)k_+ k_-$				$k = (k_x, k_y, k_z)$ $k_{\pm} = k_x \pm i k_y$	$hh \uparrow$
$ ^3/2, -^1/2\rangle$	$\frac{1}{\sqrt{6}} P k_+$	$-\frac{\sqrt{3}}{2} \beta k_+^2$ $-i 2 \sqrt{\frac{2}{3}} \mu k_- k_z$	$-\frac{1}{2}(\gamma_1 + 2\gamma_3)k_z^2$ $-\frac{1}{2}(\gamma_1 - \gamma_3)k_+ k_-$			$\mu = \frac{1}{2}(\gamma_2 - \gamma_3)$	$lh \uparrow$
$ ^1/2, -^1/2\rangle$	$\frac{1}{\sqrt{3}} P k_+$	$-\sqrt{\frac{3}{2}} \beta k_+^2$ $-i \frac{4}{\sqrt{3}} \mu k_- k_z$	$\frac{\sqrt{2}}{\sqrt{3}} \gamma_3 k_z^2$ $-\frac{\sqrt{2}}{\sqrt{3}} \gamma_3 k_+ k_-$	$-\frac{1}{2} \gamma_1 k^2 - \Delta$			$so \uparrow$
$ ^1/2, -^1/2\rangle$	0	0	$-\sqrt{\frac{2}{3}} P k_z$	$(F + \frac{1}{2})k^2 + E_G$			$c \downarrow$
$ ^3/2, -^3/2\rangle$	0	0	$\sqrt{3} \alpha k_+ k_z$ $+ i \sqrt{\frac{2}{3}} \mu k_-^2$	$\frac{1}{\sqrt{2}} P k_+$	$-\frac{1}{2}(\gamma_1 - 2\gamma_3)k_z^2$ $-\frac{1}{2}(\gamma_1 + \gamma_3)k_+ k_-$		$hh \downarrow$
$ ^3/2, +^1/2\rangle$	$\sqrt{\frac{2}{3}} P k_z$	$-\sqrt{3} \alpha k_+ k_z$ $-i \sqrt{\frac{2}{3}} \mu k_-^2$	$-\frac{3}{\sqrt{2}} \alpha k_+ k_z$ $+ i \mu k_+^2$	$\frac{1}{\sqrt{6}} P k_-$	$-\frac{\sqrt{3}}{2} \beta k_-^2$ $+ i 2 \sqrt{\frac{2}{3}} \mu k_+ k_z$	$-\frac{1}{2}(\gamma_1 + 2\gamma_3)k_z^2$ $-\frac{1}{2}(\gamma_1 - \gamma_3)k_+ k_-$	$lh \uparrow$
$ ^1/2, +^1/2\rangle$	$-\frac{1}{\sqrt{3}} P k_z$	$\sqrt{\frac{3}{2}} \alpha k_+ k_z$ $+ i \frac{1}{\sqrt{3}} \mu k_-^2$	0	$\frac{1}{\sqrt{3}} P k_-$	$-\sqrt{\frac{3}{2}} \beta k_-^2$ $+ i \frac{4}{\sqrt{3}} \mu k_+ k_z$	$\frac{\sqrt{2}}{\sqrt{3}} \gamma_3 k_z^2$ $-\frac{\sqrt{2}}{\sqrt{3}} \gamma_3 k_+ k_-$	$so \uparrow$
	$ ^1/2, +^1/2\rangle$	$ ^3/2, +^1/2\rangle$	$ ^1/2, -^1/2\rangle$	$ ^1/2, -^1/2\rangle$	$ ^3/2, -^1/2\rangle$	$ ^3/2, +^1/2\rangle$	$ ^1/2, +^1/2\rangle$

Table A.5: The 8-band magnetic field bulk $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian for the $[001]$ and $[111]$ orientations. The upper triangle is the Hermitian conjugate of the lower triangle.

	n $c \uparrow$	$n-1$ $hh \uparrow$	$n+1$ $lh \downarrow$	$n+1$ $so \downarrow$	$n+1$ $c \downarrow$	$n+2$ $hh \downarrow$	n $lh \uparrow$	n $so \uparrow$
$ \frac{1}{2}, +\frac{1}{2}\rangle$	$(F + \frac{1}{2})k_z^2 + 2(F + \frac{1}{2})(n + \frac{1}{2})B + \frac{1}{2}B + E_G$							
$ \frac{3}{2}, +\frac{3}{2}\rangle$	$P\sqrt{Bn}$	$-\frac{1}{2}(\gamma_1 - 2\gamma_x)k_z^2 - (\gamma_1 + \gamma_x)(n - \frac{1}{2})B - \frac{3}{2}B\kappa B$						
$ \frac{3}{2}, -\frac{1}{2}\rangle$	$-\frac{1}{\sqrt{3}}P\sqrt{B(n+1)}$	$-\beta B\sqrt{3n(n+1)}$	$-\frac{1}{2}(\gamma_1 + 2\gamma_x)k_z^2 - (\gamma_1 - \gamma_x)(n + \frac{3}{2})B + \frac{1}{2}B\kappa B$					
$ \frac{1}{2}, -\frac{1}{2}\rangle$	$\sqrt{\frac{2}{3}}P\sqrt{B(n+1)}$	$-\beta B\sqrt{6n(n+1)}$	$-\sqrt{2}\gamma_x k_z^2 - \sqrt{\frac{1}{2}}B\kappa B$	$-\frac{1}{2}\gamma_1 k_z^2 - \gamma_1(n + \frac{3}{2})B + \kappa B - \Delta$				
$ \frac{1}{2}, -\frac{1}{2}\rangle$	0	0	$-\sqrt{\frac{2}{3}}P k_z$	$\frac{1}{\sqrt{3}}P k_z$	$(F + \frac{1}{2})k_z^2 + 2(F + \frac{1}{2})(n + \frac{3}{2})B - \frac{1}{2}B + E_G$			
$ \frac{3}{2}, -\frac{3}{2}\rangle$	0	0	$\alpha\sqrt{6B(n+2)}k_z$	$-\alpha\sqrt{3B(n+2)}k_z$	$-\frac{1}{2}(\gamma_1 - 2\gamma_x)k_z^2 - (\gamma_1 + \gamma_x)(n + \frac{5}{2})B + \frac{3}{2}B\kappa B$			
$ \frac{3}{2}, +\frac{1}{2}\rangle$	$\sqrt{\frac{2}{3}}P k_z$	$-\alpha\sqrt{6Bn}k_z$	0	$-3\alpha\sqrt{B(n+1)}k_z$	$\frac{1}{\sqrt{3}}P\sqrt{B(n+1)}$	$-\frac{1}{2}(\gamma_1 + 2\gamma_x)k_z^2 - (\gamma_1 - \gamma_x)(n + \frac{1}{2})B - \frac{1}{2}B\kappa B$		
$ \frac{1}{2}, +\frac{1}{2}\rangle$	$-\frac{1}{\sqrt{3}}P k_z$	$\alpha\sqrt{3Bn}k_z$	$3\alpha\sqrt{B(n+1)}k_z$	0	$-\sqrt{\frac{2}{3}}P\sqrt{B(n+1)}$	$-\sqrt{2}\gamma_x k_z^2 - \sqrt{2}\gamma_x(n + \frac{3}{2})B - \sqrt{\frac{1}{2}}B\kappa B$	$-\frac{1}{2}\gamma_1 k_z^2 - \gamma_1(n + \frac{1}{2})B - \kappa B - \Delta$	
	$ \frac{1}{2}, +\frac{1}{2}\rangle$	$ \frac{3}{2}, +\frac{3}{2}\rangle$	$ \frac{3}{2}, -\frac{1}{2}\rangle$	$ \frac{1}{2}, -\frac{1}{2}\rangle$	$ \frac{1}{2}, -\frac{1}{2}\rangle$	$ \frac{3}{2}, -\frac{3}{2}\rangle$	$ \frac{3}{2}, +\frac{1}{2}\rangle$	$ \frac{1}{2}, +\frac{1}{2}\rangle$

Table A.6: All parameters used in the calculations. Where possible, experimentally determined parameters have been used.

Parameter	InAs	GaSb	InSb	GaAs
Lattice Constant (Å)	6.0584	6.0954	6.4794	5.6533
Pseudopotential Form Factors (Ryd)*				
V_3^S	-0.23	-0.22	-0.20	-0.23
V_8^S	0.0	0.0	0.0	0.01
V_{11}^S	0.045	0.05	0.04	0.06
V_3^A	0.055	0.06	0.06	0.07
V_4^A	0.045	0.05	0.05	0.05
V_{11}^A	0.01	0.01	0.01	0.01
<i>k</i> · <i>p</i> Parameters				
Band Gap E_G (meV)	418	810	235	1518
Spin-Orbit Splitting Δ (meV)	380	775	805	340
F	-0.25	-0.17	-0.25	-0.09
γ_1	1.97	2.58	2.33	1.21
γ_2	-0.48	-0.58	-0.78	-0.72
γ_3	0.44	0.65	0.52	0.08
κ	1.17	1.43	1.58	-1.62
$E_P = 2 P^2$ (eV)	22.2	22.4	23.1	25.7
Dielectric Constant ϵ_s	15.15	15.69	16.8	12.53
m_e^* (m_0)	0.023	0.042	0.014	0.0665
m_{hh}^* (m_0) [001]	0.41	0.28	0.34	0.48
m_{hh}^* (m_0) [111]	0.41	0.36	0.45	0.57
m_{lh}^* (m_0)	0.025	0.05	0.022	0.088
Elastic Coefficients (Mbar)				
C_{11}	0.8329	0.8842	0.6576	1.2114
C_{12}	0.4526	0.4026	0.3565	0.5482
C_{44}	0.3959	0.4322	0.2983	0.6042
Deformation Potentials (eV)				
a_C	-5.08	-6.85	-6.17	-7.17
a_V	1.00	0.79	0.36	1.16
b	-1.8	-2.0	-2.1	-1.7
d	-3.6	-4.8	-5.0	-4.5
Piezoelectric constant e_{14} (10^{-6} C/cm ²)	4.59	12.6	7.17	16

* 1 Rydberg (Ryd) = 0.5 Hartree = 13.6056 eV

