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GRADUATE COLLEGE

**AN INVESTIGATION OF THE PROPERTIES
OF $\text{InSb}/\text{Al}_x\text{In}_{1-x}\text{Sb}$ QUANTUM WELLS**

A Dissertation

SUBMITTED TO THE GRADUATE FACULTY

in partial fulfillment of the requirements for the

degree of

DOCTOR OF PHILOSOPHY

By

**FRED B. BROWN, II
NORMAN, OKLAHOMA
2002**

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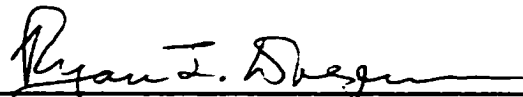
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**A Dissertation APPROVED FOR THE DEPARTMENT OF
PHYSICS AND ASTRONOMY**

BY



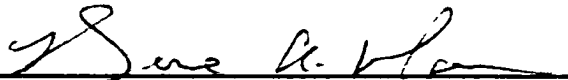
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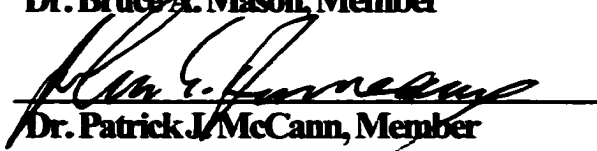
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Chapter 1: Introduction

Semiconductors have influenced the everyday lives of people around the world since the advent of the bipolar transistor in 1947. This could arguably be called the dawn of the Information Age in light of the advances this technology has made possible in electronic devices. There are many more devices available today than a generation ago, and while the complexity of design has increased, size and real cost have decreased. The vacuum tube radio cannot be produced on the scale of microprocessors, which use epitaxial and lithographic techniques in their manufacture. Despite the exorbitant cost of a production facility, microprocessors are ubiquitous aspects of daily lives. From home electronics and telecommunications to power distribution, they are everywhere. This evolution of - and dependence on - electronics is a direct result of the study of semiconductors and their physical properties.

Semiconductors can be defined alternatively as materials with resistivity between that of metals and insulators ($\rho = 10^{-3} \Omega cm$ to $\rho = 10^8 \Omega cm$) [1] or with carrier densities between $n = 10^{13} cm^{-3}$ and $n = 10^{18} cm^{-3}$ [2]. The carriers are negatively charged electrons in the conduction band and positively charged holes in the valence band. The separation in energy between the bottom of the conduction band and the top of the valence band is the band gap, E_g . Some typical band gaps are given in Table 1-1.

With the advent and refinement of epitaxial growth techniques such as Molecular Beam Epitaxy (MBE) - to be discussed later - it has become possible to “engineer” band gaps and design semiconductors with specified electrical and optical properties. The degree to which these properties can be designed into a specific material system is not infinite, however. The predominant semiconductors in application today are silicon and gallium arsenide. At room temperature their band gaps are 1.11 eV and 1.43 eV, respectively. This dissertation details the study of indium antimonide, a low band gap material (0.17 eV [3]), with unique properties that may make it an attractive alternative for electronic devices in the future.

Specifically, this work investigates $InSb/Al_xIn_{1-x}Sb$ quantum wells. In this system, the $Al_xIn_{1-x}Sb$ material has a higher band gap than $InSb$. When a thin layer of $InSb$ well material is sandwiched between two layers of $Al_xIn_{1-x}Sb$ barrier material, the carriers can be trapped in the lower energy well region. While they are free to move in two dimensions, the potential barrier of the higher band gap $Al_xIn_{1-x}Sb$ restricts motion in that third dimension. As long as the thickness of the well layer is smaller than, or on the order of, the electron wavelength, it can be said that the carriers are confined to two dimensions. As a result, the physically allowable energy levels must meet boundary conditions and are therefore discrete. The electrons and holes can form hydrogenic bound states called excitons. These states can be studied through the use of transmission spectroscopy. The details of Fourier Transform Infrared

(FTIR) Spectroscopy will be given in a Chapter 5. FTIR has proven to be a powerful technique for the study of quantum well systems.

In addition to briefly examining excitonic transitions in undoped square wells, this work will cover a detailed investigation into the determination of the band offset in the $InSb / Al_xIn_{1-x}Sb$ quantum well system. By determining the difference between the barrier band gap and the well band gap one gets, $E_{g'} - E_g = \Delta E_g$. This is the sum of the valence and conduction band barriers. What one cannot tell from this, or from direct measurement, is how much of this space is taken up by the conduction band well and how much by the valence band. It is important to know this value both from an engineering and a theoretical point of view as it can significantly affect the number of electron-hole transitions available.

Another important parameter (actually two) investigated is the deformation potential. As can be seen in Table 1-1, $AlSb$ and $InSb$ have different lattice constants ($AlSb$ being $\sim 5\%$ smaller). $Al_xIn_{1-x}Sb$ has a lattice constant between the two, which depends on the aluminum concentration (assuming a linear dependence on Al concentration, Vegard's law applies). With mismatched lattice constants, either the well or the barrier will be strained, depending on how the system is grown. The well is under compressive strain in nearly all of these systems, introducing a shift in transition energies compared to unstrained systems. Deformation potential is particularly important in modeling light hole transitions, which are strongly dependent on strain.

The above investigations all involve nominally undoped quantum well systems.

When n-type dopants are selectively added to the system the Fermi level can be raised to the point where it begins to fill the conduction subbands. When this occurs, valence to conduction band transitions in the partially filled subbands are shifted to higher energies due to the occupation of lower energy states by the excess electrons. These higher energy transitions occur at the Fermi level and are known as Fermi Edge Singularities (FES).

Chapter 2 of this dissertation will discuss the necessary background material for later chapters – the basics of quantum wells and optical interactions. A more specific treatment will be given to the properties of *InSb* in Chapter 3 - to include band structure, non-parabolicity and other parameters. Sample growth and preparation will be discussed in Chapter 4. Analysis of data and the equipment used will be covered in Chapter 5. Some experimental details will be brief, such as High Resolution X-Ray Diffraction which is used to ensure that quantum wells are fully strained. More detail will be given about FTIR spectroscopy - both theoretical and practical - as it was the primary experimental technique used in studying the valence to conduction band transitions necessary in examining the above situations. A detailed study of the dependence of the barrier band gap on temperature and aluminum concentration, band offset, deformation potential, and Fermi Edge Singularity will follow in Chapters 6 through 9, respectively. A brief summary of this research will end this dissertation in Chapter 10.

Table 1-1 Properties of Commonly Used Semiconductors

	$E_g(eV)$	m_e^*	m_{Δ}^*	m_{Σ}^*	$a(\text{\AA})$
Si	1.12		.16	.5	5.431
GaAs	1.43	.067	.074	.5	5.653
InSb	.236	.014	.015	.4	6.479
AlSb	1.63	.12			6.136

Chapter 2: BACKGROUND

Prior to the presentation of the experimental observations, a brief overview of semiconductor and quantum well fundamentals is presented. It begins with a discussion of band structure and reviews a perturbation technique for determining its form at points of high symmetry. This is followed by a study of optical absorption spectra, which is then related to the electron density of states (DOS) in bulk materials. A comparison of the three dimensional DOS with that in two dimensions leads to an examination of the properties of quantum wells. Most pertinent to this work is the physics of III-V compound semiconductors. Where useful in exemplifying a concept, results from observations on Gallium Arsenide - the most extensively studied and best understood of these materials - will be presented.

The behavior of electrons in semiconductors is described in terms of the band structure of the particular material system. These energy bands arise from the electron orbitals of the individual atoms in the material. Progressing from individual atoms to a crystal of many unit cells, the orbitals broaden into continuous energy bands. A simplified band diagram of a III-V material (e.g. *GaAs* or *InSb*) is depicted in Figure 2-1 [4]. At absolute zero in the absence of doping, the conduction band is empty of electrons while the valence bands are completely filled. In such a situation, even a semiconductor cannot conduct. However, at finite temperatures some electrons in the valence band are thermally excited into the conduction band,

leaving vacant states, or holes, behind. These conduction electrons and valence holes can conduct under the influence of an electric field.

Of more interest for the purpose of this work is the optical excitation of valence electrons to the conduction band. Many factors affect the energies at which this can occur. As a preliminary step, a model of the band structure is required for the material of interest. One technique for calculating the band structure near band edges of direct gap semiconductors is the $\vec{k} \cdot \vec{p}$ [5] method. In this region, the wave vector, $\vec{k}$, differs only slightly from some $\vec{k}_0$. Following the description of the electron in a periodic potential - such as is experienced in a crystal lattice - the wave function can be described in terms of the Bloch function as:

$$\Psi_{nk}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{nk}(\vec{r})$$

Equation 2-1

where $u_{nk}(\vec{r} + \vec{R}) = u_{nk}(\vec{r})$. For an electron in a periodic potential, $V(\vec{r})$ (as experienced in a crystal lattice), one starts with the time independent Schrödinger equation and substitutes in the Bloch function for Ψ_{nk} , providing:

$$\left[\frac{p^2}{2m_0} + \frac{\hbar}{m_0} \vec{k} \cdot \vec{p} + V(\vec{r}) \right] u_{nk}(\vec{r}) = \left[E_n(\vec{k}) - \frac{\hbar^2 k^2}{2m_0} \right] u_{nk}(\vec{r})$$

Equation 2-2

When solved for a single band about $\vec{k}_0 = 0$, this provides the conduction band as seen in Figure 2-2a [4]. Modification to solve for two bands can be achieved by assuming:

$$u_{nk}(\vec{r}) = \sum_n a_n(\vec{k}) u_{n0}(\vec{r})$$

Equation 2-3

giving the conduction and heavy hole valence bands shown in Figure 2-2b. Of more practical interest is when spin-orbit interactions are considered in the Hamiltonian

through the inclusion of the following term: $\frac{\hbar}{4m^2c^2} [\nabla V \times \vec{p}] \cdot \vec{\sigma}$, where the $\vec{\sigma}$ are the

Pauli spin matrices. The Schrödinger equation then becomes:

$$\left[\frac{p^2}{2m_0} + V(\vec{r}) + \frac{\hbar}{m_0} \vec{k} \cdot \vec{p} + \frac{\hbar^2}{4m_0^2c^2} [\nabla V \times \vec{p}] \cdot \vec{\sigma} + \frac{\hbar^2}{4m_0^2c^2} \nabla V \times \vec{k} \cdot \vec{\sigma} \right] u_{nk}(\vec{r}) = [E_n(\vec{k}) - \frac{\hbar^2 k^2}{2m_0}] u_{nk}(\vec{r})$$

Equation 2-4

Ignoring the last term on the left as a small crystal momentum term (compared to the atomic momentum terms) yields 8 functions for $u_{n0}(\vec{r})$: 2 spin 1/2 states for the conduction band and 6 spin 3/2 states for the valence band which correspond to four bands (conduction, heavy hole, light hole, and split off spin-orbit bands). These bands are depicted in Figure 2-3 [4].

Next is an examination of optical absorption. The upper curve in Figure 2-4 [6] is an absorption spectrum for bulk *GaAs*. Note that for energies below the band gap of *GaAs* (1.43 eV) there is no absorption. Near the band gap energy, there is an abrupt

onset of absorption. It is here that the photons absorbed by the valence electrons have enough energy to be excited into the conduction band.

There is a strong resemblance between this absorption spectrum and the predicted 3D density of states shown in Figure 2-5 [7]. This similarity is consistent as empty states must be available to allow photons to promote the electrons through absorption. If no states are available, the photon will not be absorbed. One significant difference in the absorption spectrum is the sharp peak at onset. This occurs slightly below the band gap and is due to the formation of hydrogenic bound states between the electrons and holes, called excitons. The observation of what energies exciton peaks occur at is useful in determining some characteristics of the materials being observed and is used extensively in this work.

Excitons are observed in 2D systems as well. To form a Type I quantum well out of semiconducting materials, a layer of lower band gap material (the well) must be sandwiched between layers of a higher band gap material (the barrier). When the well is thin enough (on the order of the electron wavelength) the density of states takes on a step-like structure. Figure 2-5 also shows the ideal 2-D density of states. This confinement in one dimension quantizes the available energy levels and can be observed in absorption spectroscopy. Many interesting features besides the stepped plateaus are observed, as shown in the transmission spectrum in Figure 2-6. These peaks, with sharp onsets occurring slightly below where the density of states would suggest, are excitons formed as electrons are excited from the valence band to the

conduction band. Bulk, or 3D, semiconductors typically show one exciton peak. In quantum wells, however, the energy levels of the conduction and of the valence bands are quantized and multiple exciton peaks may be observable, both for heavy and light hole transitions.

In an ideal square quantum well with infinite barriers, transitions to a specific conduction subband with index “n” would only occur from the valence subband with the same index. This is due to the orthogonality of all wavefunctions with different indices, so that the transition matrix element would be zero. This orthogonality is graphically represented in Figure 2-7 [8]. In the practice, barriers are not infinite, wells are not perfectly square and bands are not truly parabolic. This means that the wavefunctions are not strictly orthogonal and transitions between subbands of different index may occur. These “forbidden” transitions can provide valuable additional information about the band structure of the material.

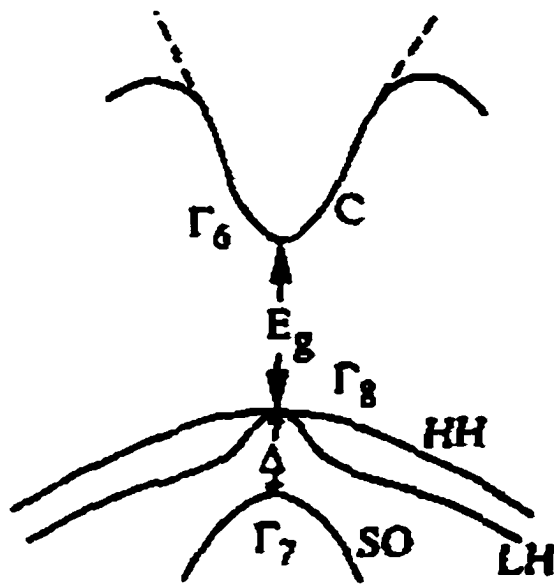


Figure 2-1 Band Diagram

Simplified bulk band diagram for typical III-V compound semiconductors[4].

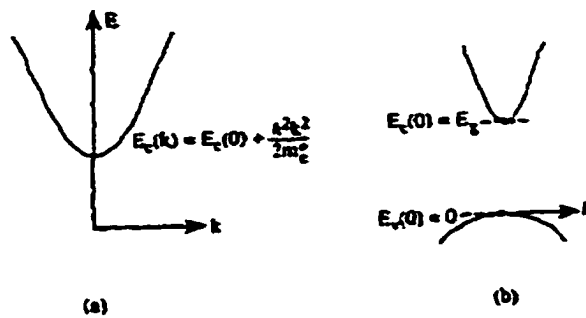


Figure 2-2 Simple Models

One and two band models [4].

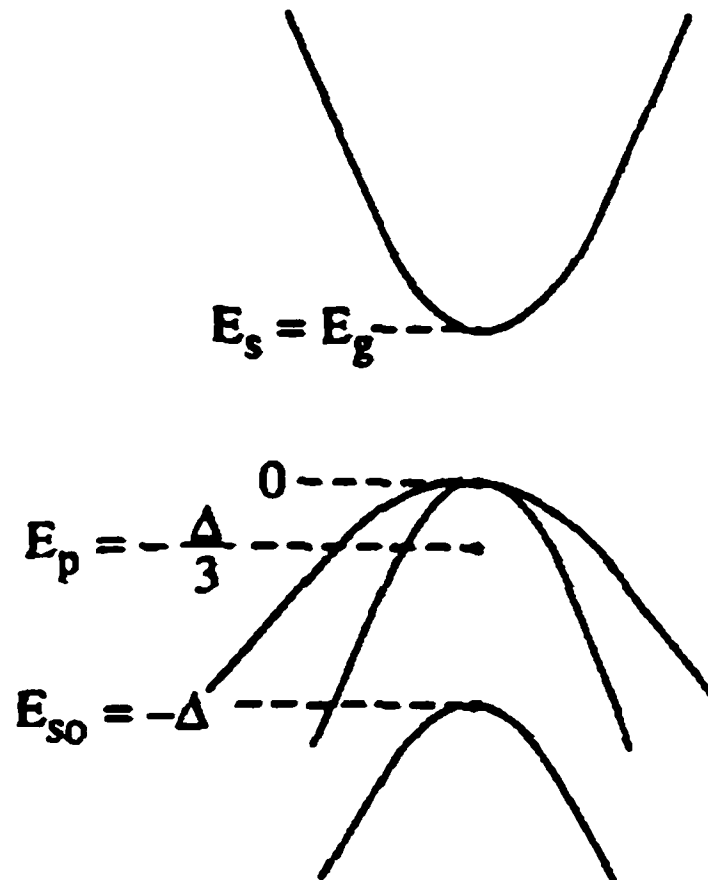


Figure 2-3 Four Band Model

A more complete four band model [4].

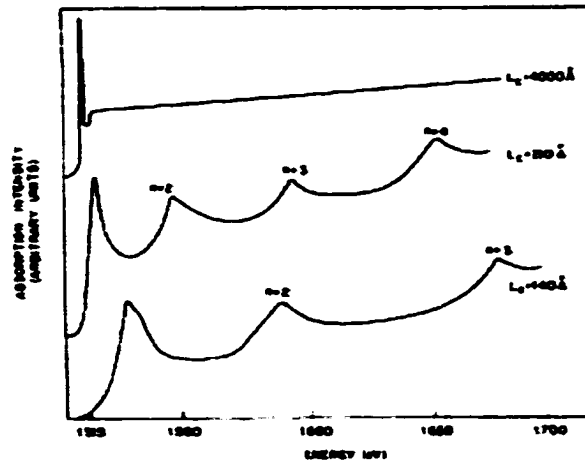


Figure 2-4 Absorption in GaAs

Spectra showing confinement effects in GaAs. L_z is the layer thickness of the GaAs [6].

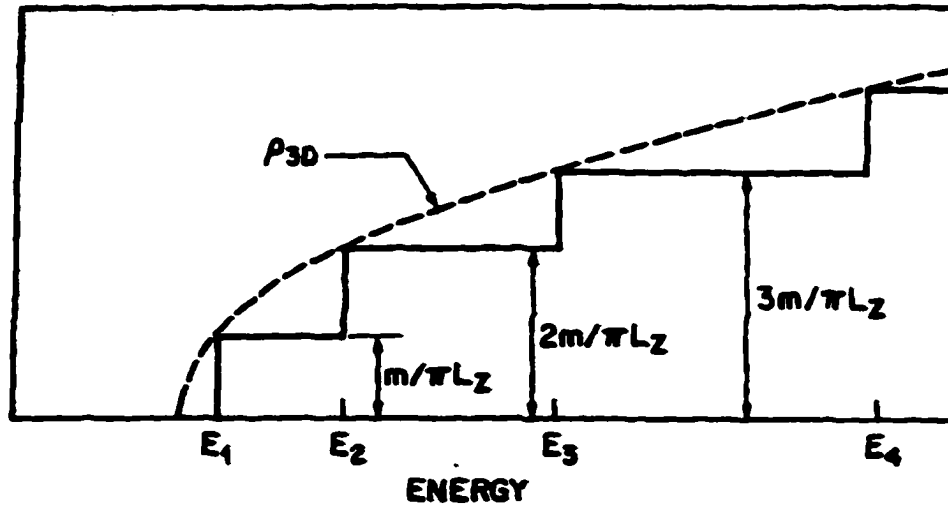


Figure 2-5 Theoretical Density of States, 2D versus 3D

Theoretical density of states (DOS) for the 2D and 3D cases. The 3D DOS exhibits a sharp onset followed by a continuous increase. The 2D DOS exhibits a step-like increase [7].

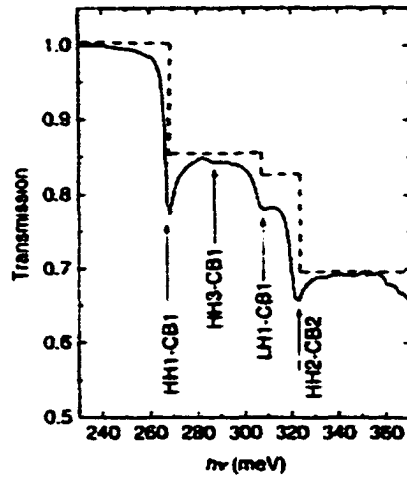


Figure 2-6 Transmission Spectrum of InSb

Spectrum of sample S595 demonstrating the step-like structure due to confinement in a quantum well.

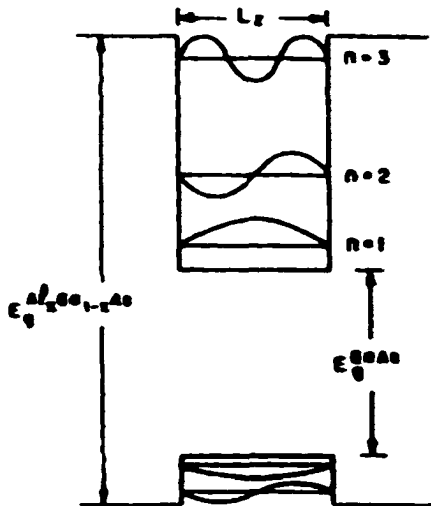


Figure 2-7 Ideal Square Well

Electron and hole wavefunctions: Due to an infinite potential (not depicted) square quantum well [8].

Chapter 3: Basic Properties of InSb

3.0 Structure

An initial discussion on the basic material and electronic properties of *InSb* is in order prior to examination of experimental results. *InSb* is a III-V material that forms in a zinc blend structure as shown in Figure 3-1 [9] for a unit cell and a series of layers. Each indium ($5s^25p$ electronic configuration) has 4 antimony nearest neighbors ($5s^25p^3$). The structure can be viewed as two FCC lattices offset by

$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a$ along the (111) direction, where a is the cubic cell edge length (lattice

constant). The lattice constant at 298K of unstrained *InSb* is $a = 6.479 \text{ \AA}$. The indium forms an sp^3 hybridized tetrahedral bond with its antimony neighbors.

Typical of III-V semiconductor materials, *InSb* has a direct energy gap at the Γ^6 point. Figure 3-2 [10] depicts the band structure of *InSb* with relevant parameters at room temperature. There are many factors that single out *InSb* among III-V binary compound semiconductors. Of particular note is the low value of energy gap. *InSb* has the smallest band gap in this group. It also has the highest intrinsic electron mobility at room temperature. Adding to this its very strong non-parabolicity in the conduction band makes *InSb* a unique material that has great potential for specialized photonic and high-speed electronic devices. Each of these factors will be addressed briefly in the remainder of this chapter.

3.1 Energy Gap

The definition of the energy gap is the separation between the top of the valence band and the bottom of the conduction band. The origin of the energy gap in semiconductors can be explained in different ways. An approach based on the chemical bonding between two like atoms explains the allowed versus forbidden energy region for valence electrons based on symmetric versus anti-symmetric bonds. As the number of atoms increases to form a solid, the allowed states form continuous bands, with the forbidden states forming an energy gap.

An alternate approach, developed by Bloch, is based on the periodic potential experienced by electrons due to the crystal lattice. In this method, the individual electrons are described by the free electron wave equation of the form, $e^{i\vec{k}\cdot\vec{r}}$, with the periodic potential of the lattice put into the Schrodinger Equation:

$$\nabla^2\Psi + \frac{2m_0}{\hbar^2}(E(\vec{k}) - V(\vec{r}))\Psi = 0$$

Equation 3-1

The solutions are known as the Bloch functions which have the form:

$$\Psi_n(\vec{k}, \vec{r}) = u_n(\vec{k}, \vec{r})e^{i\vec{k}\cdot\vec{r}}$$

Equation 3-2

This solution contains the lattice periodicity in the factor $u_n(\vec{k}, \vec{r})$ such that

$u_n(\vec{k}, \vec{r}) = u_n(\vec{k}, \vec{r} + \vec{T})$, where $\vec{T}$ is a translation of a lattice vector. The energy

bands are the linear combination of these waves, with the index n specifying the band. Real solutions for these equations yield forbidden energy regions, which give rise to the energy gap.

In pure bulk *InSb*, the energy gap is direct at the Γ point, meaning that the minimum in energy of the conduction band occurs at the same place as the maximum in the valence band. The value of this direct gap ranges from approximately 236meV at 0K to 180meV at room temperature. This variation of energy gap with temperature is approximately quadratic at lower temperatures and linear at higher temperatures and is discussed in detail in Chapter 6. Other factors that can affect the value of the energy gap are strain, confinement, and alloy composition, each of which is discussed in later chapters.

3.2 Non-parabolicity

The narrow band gap of *InSb* – along with the small effective masses of the electrons and light holes – results in strong coupling between the valence and conduction bands. The result of this is a strong non-parabolicity in the conduction and light hole bands as one moves away from the zone center. Early absorption spectra of *InSb* taken by Gobeli and Fan [11] indicated inconsistencies in a purely parabolic dispersion relation. While they did postulate the possibility of a warped light hole band, much of their discussion speculated on warping of the heavy hole band. This was due in part to inconclusive evidence at the time of the existence of light holes. The importance of band non-parabolicity to the research described in this dissertation

is that it breaks the orthogonality of different index valence to conduction band transitions in *InSb* quantum wells. This is discussed in later chapters in more detail.

3.3 Electron Mobility

Electron mobility is a measure of the ability to move electrons with an applied

electric field. It is defined as $\mu_e = \frac{|v|}{E}$, where v is the electron drift velocity. *InSb*

has the highest room temperature intrinsic electron mobility among all semiconductors with a value of $77000 \text{ cm}^2/\text{V.s}$ [12]. This high mobility is related to the small electron effective mass, which is typical of direct gap semiconductors with small energy gaps.

In bulk *InSb*, mobility exhibits a strong dependence on electron concentration, as is shown in Figure 3-3 [13] for 300K. The lowering of mobility with increasing concentration can be attributed to impurity scattering. There is also a pronounced decrease at high temperatures. The mobility peaks at 50K [12], and drops steeply above 200K (see Figure 3-4 [14]), though can still be as high as $40,000 \text{ cm}^2/\text{V.s}$ [15] at room temperature in doped materials. This mobility can be significantly increased in *InSb* quantum wells, which is discussed in Chapter 4.

3.4 Summary

The unique properties of *InSb* can be exploited for both industrial and research purposes. Its non-parabolic band structure has led to the exploration of perturbation methods for describing band structure. Similarly, high mobility is useful in exploring

the Quantum Hall Effect. Industrial applications include magnetic field sensors, mid-infrared optical devices, and high speed and low power electronic devices. Examples of optical devices are thermal imaging detectors and cameras that can operate at liquid nitrogen temperatures [16]. *InSb* based high frequency FET's and bipolar transistors have also been made [17]. Further research on the basic properties of *InSb* is ongoing in both industry and academia with the potential of better theoretical models and increased applications for the material.

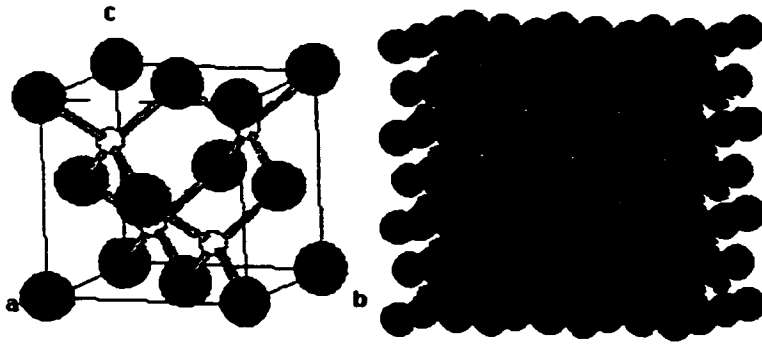


Figure 3-1 Zinc-Blend Structure

The tetrahedral bonds between indium and antimony are depicted on the left. The lattice vectors a , b , and c are equal in InSb [9].

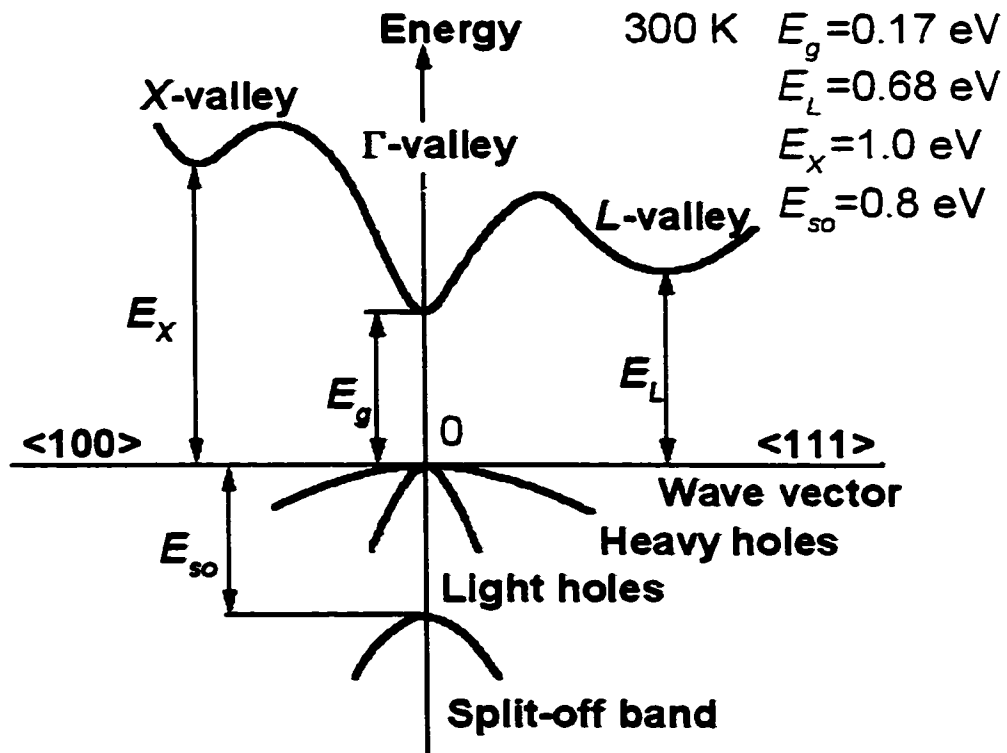


Figure 3-2 Simplified InSb Band Structure

Room temperature energy spacing between extrema in the InSb band structure [10].

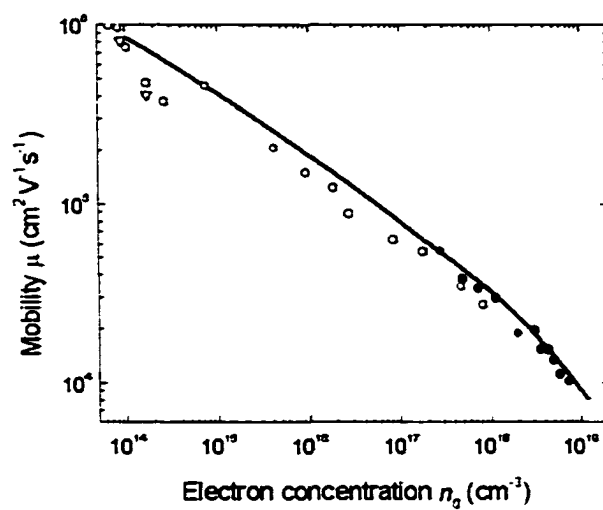


Figure 3-3 Mobility Versus Electron Concentration

Mobility versus electron concentration for InSb at room temperature [13].

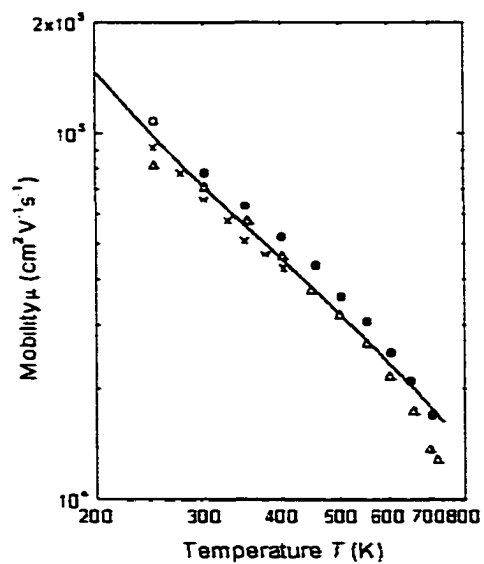


Figure 3-4 Mobility at Higher Temperatures

The electron mobility in InSb above 200K shows a sharp decrease with increasing temperature [14].

Chapter 4: Sample Preparation

4.0 Design

Indium antimonide multiple quantum wells are grown [18] by MBE on semi-insulating (001) gallium arsenide substrates after the deposition of buffer layers to alleviate strain (and allow lattice relaxation in the buffer layers) due to the large lattice mismatch between *GaAs* and *InSb* (5.653 Å and 6.479 Å , respectively at 300K). Representative examples of doped, undoped, and parabolic wells are depicted in Figure 4-1 through Figure 4-4 [19]. The final buffer layer and barrier material is $Al_xIn_{1-x}Sb$, an alloy containing the desired concentration of aluminum, x . The quantum wells are lattice matched to the alloy due to the smaller lattice constant of the alloy (alloy lattice constant is related to composition linearly via Vegard's Law). A final *InSb* capping layer is deposited to prevent oxidation of the aluminum alloy.

4.1 Characterization

Sample characterization involves a number of steps. Growth rates for *InSb* and *AlSb* are calibrated prior to crystal growth using RHEED oscillations that depict layer growth. Aluminum concentration is then deduced from growth rates [20]. This enables the growers to determine well and barrier thickness to an accuracy on the order of a monolayer. Aluminum concentration has been verified through High Resolution X-Ray Diffraction (HRXRD) and is discussed in Chapter 6. This was accomplished by identifying the separation between the peaks of the alloy and *InSb* in a rocking curve. This separation enables one to determine the alloy lattice constant

which then gives the aluminum concentration through Vegard's Law. This work (as detailed in Chapter 6) enables one to determine the aluminum concentration through transmission spectroscopy by identifying the alloy gap absorption edge. Hall effect measurements are used to determine electron concentration for doped samples as detailed by Liu, et. al.[20]. No direct measurements of interfacial roughness have been carried out on these samples, but AFM studies of sample surfaces showed defects whose frequency decreased for multiple quantum wells as opposed to single quantum wells. Mobility at 77K was significantly reduced for the single quantum well sample as opposed to the multiple quantum wells (2 - 14 well). For a single well, mobility was 126,500 cm²/Vs versus 175,500 cm²/Vs for 2 wells. AFM studies of the single well samples surface showed more abrupt step structures (height of ~100 Å) as compared with multiple well samples. These factors could indicate some roughness of the quantum well interfaces [15]. In most quantum well systems studied for this work, interface roughness has a minor effect. This is due to the fact that most of the wells are relatively thick (≥ 200 Å) and that the exciton Bohr radius is relatively large (approximately 600 Å in bulk *InSb*)

4.2 Strain and Critical Thickness

Lattice mismatch between barrier and well materials is accommodated by defects, such as dislocations, which affect heterojunction smoothness (which can propagate throughout the sample) - or by strain in either (or both) of the materials. As mentioned above, these samples are grown on *GaAs* substrates and it is the buffer layers that accommodate strain relaxation due to lattice mismatch. The composition

of the final buffer layer is what sets the lattice constant upon which all subsequent layers are grown. In many of the samples, the final buffer material is identical to the barriers. In this situation, the barrier is under no strain. Aluminum concentration determines the barrier lattice constant and is therefore a tool for controlling the amount of strain in the quantum well system. It is also possible to design the final buffer layer such that it is the barriers, rather than the wells, that are under strain. Should either of the materials be fully strained, then interfacial dislocations would ideally be eliminated. In most of this work, it is the quantum wells that are strained (some of the parabolic wells were barrier strained). So as to avoid partial relaxation of the well material, one must ensure that the quantum wells are below a critical thickness, which depends on the amount of strain they are under due to the lattice mismatch with the barrier. As long as it is below this critical thickness, the wells will match their lattice spacing to that of the barrier. A study of critical layer thickness versus aluminum concentration has been carried out by Barnett, et. al. [21] and the theoretical curve is shown in Figure 4-5. In this work, fully strained quantum wells have been grown up to 275 Å with an aluminum concentration of 9%. A fully strained 30% concentration has been attained with well thickness of 50 Å. A full discussion of strain and deformation potential will be carried out in Chapter 8.

4.3 Polishing and Final Preparation

After growth, the backs of the *GaAs* substrates were polished to increase light transmission. The samples were mounted with paraffin on a plate and attached to a South Bay Technology, Inc. polishing wheel. A 1 micron MgO Buehler Magomet

Polishing Compound was used. Polishing takes approximately 1 hour. Upon removal, the samples were cleaned in a hot methanol bath for not more than 5 minutes, followed by an acetone and de-ionized water rinse to remove all the paraffin and polishing compound.

Prior to taking data, the samples are coated with an antireflective coating to reduce Fabry-Perot interference due to the capping layer. This is accomplished by evaporating a thin film of nichrome (NiCr) on the surface under vacuum. The samples are mounted on a plate adjacent to a clean glass slide (approximately 25 mm x 20 mm). Two leads are soldered with indium to the slide so that resistance can be measured as the nichrome is deposited. NiCr is crushed and placed in a tungsten boat (obtained from R. D. Mathis Company), which is mounted to posts in an Edwards Coating System model E306A evaporator. Upon evacuation, current is slowly ramped to about 60 amps until evaporation starts. As the NiCr evaporates, measured resistance is reduced. The current is turned off and evaporation ceases when a resistance of 400 ohms is reached. Upon cooling, the samples are removed and can then be mounted in the spectrometer for observation.

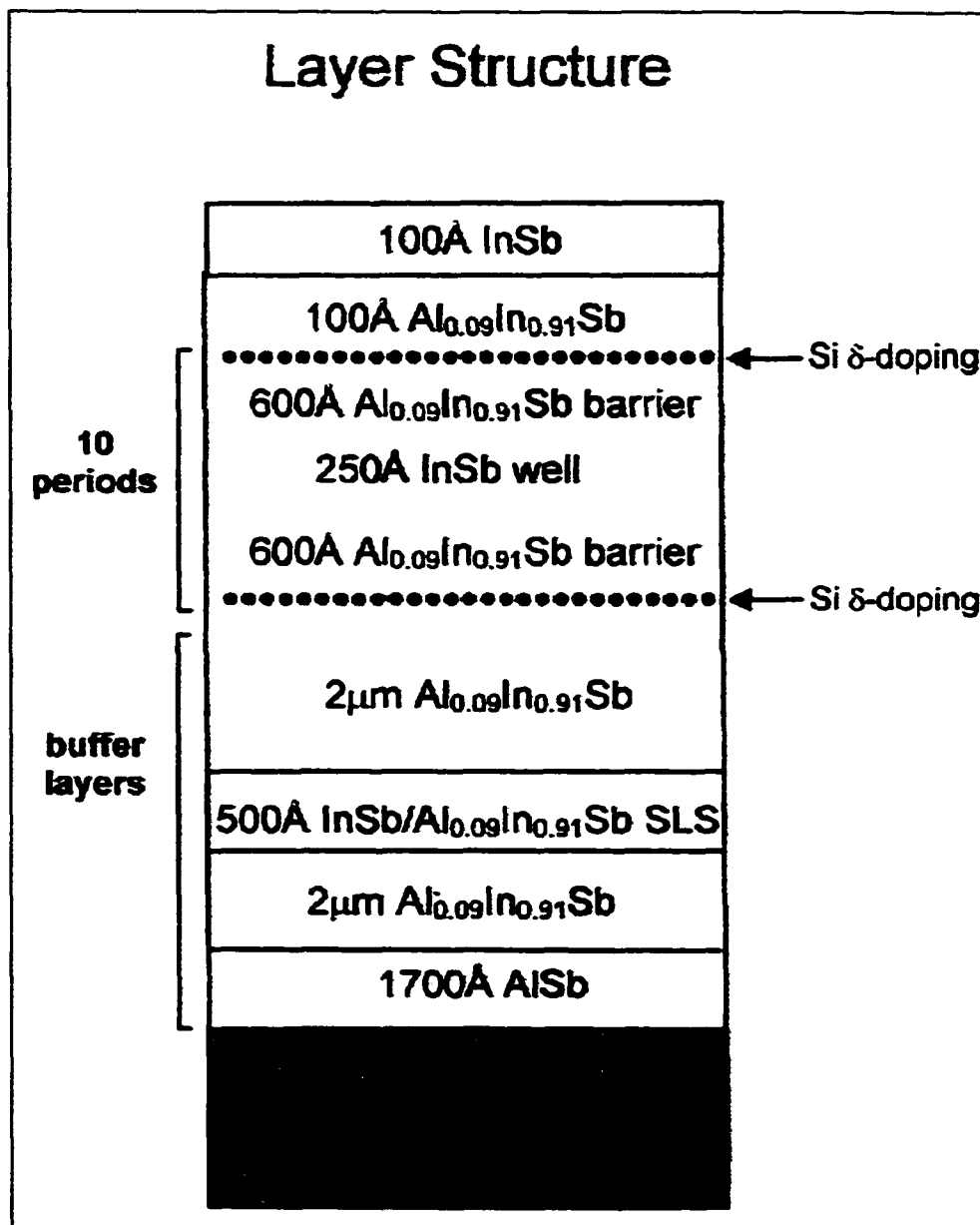


Figure 4-1 Schematic of Doped Multiple Quantum Wells

In the above figure, the buffer layers accommodate the lattice mismatch between the GaAs Substrate and the $\text{Al}_{0.09}\text{In}_{0.91}\text{Sb}$ alloy so that the barrier layers are unstrained [19].

InSb cap	100Å
10% AlInSb spacer	500Å
InSb well	50Å
10% AlInSb spacer	500Å
InSb well	50Å
10% AlInSb barrier	500Å
10% AlInSb buffer ~2μm	
10% AlInSb/InSb SLS 10×(25 Å+25 Å)	
10% AlInSb buffer ~1μm	
GaSb layer ~130Å	
AlSb Nucleation Layer 5000Å	
GaAs buffer layer ~1200Å	
GaAs (001) substrate	

Figure 4-2 Schematic of Undoped Multiple Quantum Wells

Undoped samples differ only in the absence of the silicon dopants [19].

150Å InSb cap layer
25X 7%AlInSb/InSb parabolic wells 1000Å-wells and 500Å alloy spacers
7% AlInSb layer ~2.1µm
7% AlInSb/InSb SLS 10x(25Å+25Å)
7% AlInSb layer ~1.1µm
GaSb cap ~125 Å
AlSb buffer ~0.5µm
GaAs buffer layer ~1700Å
GaAs (001) substrate

Figure 4-3 Schematic of Parabolic Quantum Well

Representative diagram of the design of a sample containing a parabolic quantum well [19].

Gr.			42	500Å	7%AlInSb spacer
1	2.375Å	InSb	41		
2	45.125Å	7% AlInSb	40		
3	9.375Å	InSb	39		
4	36.125Å	7% AlInSb	38		
5	17.875Å	InSb	37		
6	28.125Å	7% AlInSb	36		
7	25.375Å	InSb	35		
8	21.125Å	7% AlInSb	34		
9	31.875Å	InSb	33		
10	15.125Å	7% AlInSb	32		
11	37.375Å	InSb	31		
12	10.125Å	7% AlInSb	30		
13	41.875Å	InSb	29		
14	6.125Å	7% AlInSb	28		
15	45.375Å	InSb	27		
16	3.125Å	7% AlInSb	26		
17	47.875Å	InSb	25		
18	1.125Å	7% AlInSb	24		
19	49.375Å	InSb	23		
20	0.125Å	7% AlInSb	22		
21	50Å	InSb			

Figure 4-4 Detail of Digital Parabolic Profile

The details of how a parabolic well profile is digitally realized through the careful variation in the thickness of InSb and AlInSb [19].

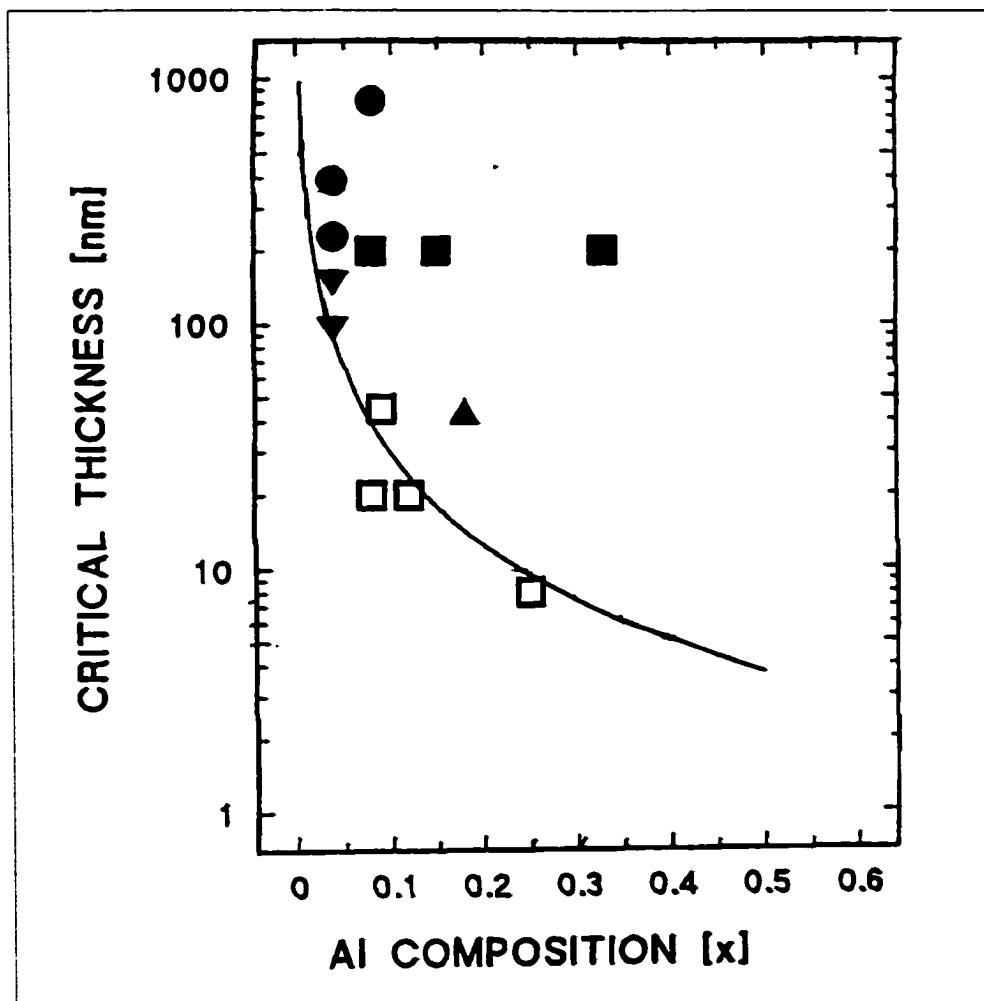


Figure 4-5 Critical Layer Thickness Versus Aluminum Concentration

The squares, circles and triangles are experimental data points. Opened squares are fully strained single layers with no misfit dislocations. The curve gives the theoretical critical thickness. All samples to the right of the curve (solid data points) had misfit dislocations [21].

Chapter 5: Experimental Details

5.0 Review of Characterization

5.0.1 Hall measurements

For studies involving doped samples, it is necessary to know the electron sheet concentration, n (cm^{-2}), so that the electron level relative to conduction subband energy at $\bar{k} = 0$ can be determined. This is accomplished by Hall measurements at room temperature, 77K, and 7K. To calculate the population level relative to subband position, the relation $k_f = \sqrt{2\pi n}$ is used, where n is the electron concentration per well and then calculate the $E(k)$ dispersion curve for the conduction subbands using a two-band approximation taking band non-parabolicity into account. Figure 5-1 is a dispersion curve for the conduction subbands for a 200 Å quantum well. In this case, for an electron concentration of $4.87 \times 10^{11} / \text{cm}^2$, the subband energy is defined using the E vs. K plot as 54meV above the bottom of the first conduction subband.

5.0.2 X-ray measurements

X-ray measurements were carried out to ensure samples are fully strained. A Philips HR-2 High Resolution Materials Research Diffractometer (MRD) was used to take area scans of the sample. This type of scan is a reciprocal space plot of the sample structure. After calibration is carried out following instructions [18], an area scan of the sample is taken. Figure 5-2 shows the theoretical alignment of the $[-1 -1 5]$ reciprocal lattice point for unstrained *GaAs*, *AlSb*, and *InSb*. The vertical axis in

the plot is parallel to the sample normal. Different positions along this axis correspond to different plane spacing. Since the three materials are unstrained, and of the same [hkl], they lie on a line that passes through the origin in reciprocal space. Different positions along this line indicate a different lattice constant. By observing the $InSb$ and $Al_xIn_{1-x}Sb$ peaks to be aligned vertically rather than along the radial axis, one can be assured that the $InSb$ quantum wells are fully strained to the lattice constant of the alloy. In Figure 5-3, which is a 21.3% aluminum sample, one sees a similar alignment, with the alloy at its unstrained lattice constant. The vertical tail downward is due to the lattice matched $InSb$ quantum wells. This tail is enlarged in Figure 5-4. Figure 5-5 shows a similar region for a 32.2% sample.

The MRD is also capable of determining aluminum concentration. It was used in this manner for work done on the temperature dependence of the alloy band gap. This work is the basis of spectroscopically determining aluminum concentration based on the absorption edge position of the $Al_xIn_{1-x}Sb$ alloy and will be more fully discussed in Chapter 6.

5.1 FTIR Fundamentals

Fourier Transform Infrared (FTIR) spectroscopy is the primary tool used in the experiments discussed in this dissertation. This section will discuss the basic theory behind the use and components of an FTIR system. Following is a discussion of the practical aspects of taking data - some particular to the system used - others associated with the techniques of spectral analysis.

5.1.1 Theory/Practice

FTIR spectroscopy is a method a wide spectrum is sampled. An understanding of the components of an FTIR system is necessary. As with any spectroscopic system, there is a source of light, a detector, and optics to guide the light. Of primary importance to an FTIR system is the inclusion of a computer controlled Michelson interferometer between the source and the detector. A beam splitter divides the source output into two beams of approximate equal intensity. One beam is reflected off of a fixed mirror, while the second is reflected from a moving mirror. The beams are then recombined before being directed through a sample to the detector. As the beams have traveled a different path length, all spectral elements interfere either constructively or destructively. This difference in path length is referred to as retardation, given in centimeters. The detector merely measures the intensity of the incident light, which varies with the retardation. Plotting this intensity versus retardation yields an interferogram.

The spectrum is obtained by relating retardation to the frequency of the incident light. This is best illustrated by considering a monochromatic source. For a constant mirror velocity, the interference maxima and minima occur every half wavelength of retardation. As the computer controls the velocity of the moving mirror, it is a known quantity, v_m (usually given in cm/s). Taking advantage of the relationship between retardation and wavelength, one relates the mirror velocity to wavelength through the relationship $v_m \tau = (\lambda/2)$, where τ is the period for the mirror to move through $\lambda/2$. The frequency of the light - being the inverse of τ - is then related to its wavenumber,

ν_{bar} , by $f=2\nu_m\nu_{\text{bar}}$. Wavenumber is the standard abscissa in IR measurement, and is related to the optical frequency, ν , by $\nu=c\nu_{\text{bar}}$.

As the incident radiation is a continuum of frequencies, the interferogram ($F(\delta)$) can be related to the optical spectrum ($T(\bar{\nu})$) by a standard Fourier Transform:

$$F(\delta) = \int_{-\infty}^{\infty} T(\bar{\nu}) e^{i2\pi\delta\bar{\nu}} d\bar{\nu}, \quad T(\bar{\nu}) = \int_{-\infty}^{\infty} F(\delta) e^{-i2\pi\delta\bar{\nu}} d\delta.$$

Realistically, the mirror can be driven only over a finite range (on the order of centimeters in practice) and the detector takes a reading over some nonzero retardation interval. The net result is that resolution is limited by these factors and can be shown to be δ^{-1} .

5.1.2 Equipment

A Bio-Rad model FTS 60-A spectrometer is used in all optical measurements. It is equipped with two sources. A globar provides mid-infrared radiation - the range of interest in these studies. It also has a mercury ion lamp for far infrared illumination.

These sources are water cooled so as to prevent misalignment due to thermal expansion of optical components. It is equipped with two detectors - a DTGS (deuterated triglycine sulfate) room temperature detector and a MCT (mercury cadmium telluride) liquid nitrogen cooled detector. Dry nitrogen is used for the air bearings of the moving mirror and to purge the spectrometer of all water vapor.

A KBr (potassium bromide) beam splitter is mounted inside the optics compartment of the spectrometer. A He-Ne laser is used to dynamically align the beam splitter.

The laser light passes through the interferometer and falls on three intensity detectors,

which detect the interference fringes. A feedback system ensures alignment of the beam splitter through piezoelectric feedback. The laser is also used to measure change in retardation and ensure that the interferogram is sampled at set intervals.

Upon recombination of the two beams, the light is directed through a sample chamber at the front of the spectrometer prior to reaching the detector. A Cryo Industries model CRC110C cryostat is mounted in the sample area. The mount is adjustable to ensure that the sample is in the beam path. Samples are mounted in the cryostat, which is then evacuated prior to cooling the sample. Sample spectra are taken at temperatures ranging from room temperature down to 4.2K. Temperature is measured through connection to a Lakeshore Cryotronics, Inc. model DRC-93C temperature controller. Below 77K, temperature is controlled by a flow rate valve in the liquid helium transfer tube. This has been found to provide better temperature stabilization than the heater in the cryostat.

5.1.3 Specific issues/considerations

It is best to keep the spectrometer on at all times for a number of reasons. Upon first turning on the spectrometer, it takes approximately four hours for the optics to stabilize in temperature. The sources are continually cooled for this reason. The system is continuously purged with dry nitrogen gas as humidity can damage the optics and will destroy the KBr beam splitter. Should the dry nitrogen be turned off, it is essential that the beam splitter is placed in a dry environment and that the cooling water be turned off.

The manufacturer recommends that the beam splitter never be manually aligned. Unfortunately that was not possible, even with a new beam splitter. Care must be taken in manual alignment and it is best to avoid if possible. Detailed steps are outlined in Appendix A.

An additional step taken is to block the He-Ne laser beam from illuminating the sample compartment. To accomplish this an undoped silicon wafer is used since it is transparent to the IR radiation in the regions of interest in these experiments. This eliminates the possibility of any unwanted excitations in the samples due to the laser. Another concern with the laser is at the three laser detectors. It has happened that the intensity of the beam was too strong for the AD converter. When this happened, laser intensity was reduced only at the detectors by placing a piece of colored glass in front of the detectors. This in no way interacts with the IR light illuminating the sample.

A parameter file is used to set up specific requirements for each spectrum taken. This is where the scan name, number of scans, resolution, and source are specified. A sample file is listed in Appendix B. It is important to keep these parameters consistent between different scans that are to be compared. Scripts for converting data to ascii are listed in Appendix C.

5.2 Method Analysis

Analysis of spectra is carried out in two ways. Transmission spectroscopy is used to determine aluminum concentration. Background spectra of *GaAs* substrates have been taken at numerous temperatures (4.2K, 77K, etc.). By taking a ratio of the

sample spectrum to the background, the alloy gap absorption edge is clearly identified. Identifying the high energy inflection point of this portion of the spectrum enables one to determine the alloy band gap. The inflection point is determined by taking a derivative of the spectrum and locating the minimum of the curve. Figure 5-6 depicts the transmission spectrum of a 50 Å MQW sample and its derivative. The exciton transitions and alloy gap absorption edge are clearly identifiable in the derivative spectrum and are highlighted by the vertical lines to the same transitions in the transmission spectrum.

The analysis of the sample spectra can also be accomplished via transmission spectroscopy. Figure 5-7 depicts just such an analysis, with 3 identified transitions. Note that the light hole transition is weak and it would be difficult to unambiguously pick its location. Rather than use this method, this research takes advantage of the strong temperature dependence of the *InSb* and alloy band gaps. The raw spectra of the same 250 Å undoped sample as in Figure 5-7 is shown in Figure 5-8 at 4K and 30K. There is minimal difference between the spectra at different temperatures except at the energies corresponding to interband exciton transitions. By taking the difference between these two spectra, only those regions where the spectrum is significantly altered are enhanced. This is demonstrated in Figure 5-9, which exhibits sharper features than the same sample in Figure 5-7. This identifies the interband transition energy as the high energy inflection point, as is done for the band gap. An additional benefit of this method is that samples do not need to be changed between data runs. In other words, the spectra being compared are taken under identical

conditions, barring temperature (e.g. calibration of electronics and radiation angle of incidence are unchanged). Care must be taken when choosing the temperatures for which to take a difference. Below 77K, the band gap of *InSb* varies by less than 10meV. In this temperature range, a difference of ~20K-25K yields sharp features. At higher temperatures, the variation of band gap with temperature is much larger, requiring a smaller temperature difference so as to not smear out the transitions. Figure 5-10 compares the difference spectrum in Figure 5-9 with one at higher temperatures (50K - 77K). While the features are still clearly identifiable, one can see that they are broader at the higher temperatures. A full discussion of the temperature dependence of band gap is carried out in the next chapter.

5.3 Observation of Excitons

Optical spectroscopy has been extensively used in the observation of interband transitions for many material systems. These experiments on *InSb/Al_xIn_{1-x}Sb* multiple quantum wells have resulted in the observation of interband exciton transitions in many samples. As with the above discussion on spectral analysis, this section will focus primarily on the spectrum of sample S595. Excitons have been detected over a wide range of quantum well conditions. Well widths have varied from 50 Å to 375 Å for square well samples. The degree of strain in the quantum wells ranged from fully strained to partially strained to fully relaxed. Additional experiments were carried out on parabolically graded quantum wells. In each of these cases, strong exciton spectra were observed.

The transmission spectrum at 4.2K of S595 is shown in Figure 5-7. This sample is a 250 Å MQW with 25 wells separated by 500 Å barriers. It is nominally undoped with an aluminum concentration of ~9%. The sample spectra exhibit the characteristic step-like structure associated with a two dimensional density of states, represented by the dashed line in the figure. Excitonic continuum absorption features are also seen at each step. Figure 5-9 is of the same energy range, with sharper features as discussed above. The exciton peaks are labeled by which valence subband the electron was excited from and by the conduction subband it was excited to (i.e. a transition from the first heavy hole subband to the first conduction subband is labeled as HH1-CB1). The transitions observed are H1-CB1, HH2-CB2, HH3-CB1, and LH1-CB1. Assignments were made by comparison of predicted transition energies. Calculations accounted for strain in the system and used a two-band model with (non-parabolicity) for the conduction and light hole bands (calculations using a four band model have also been used with consistent results). The heavy hole band was approximated to good degree as parabolic. These calculations predicted two conduction subbands, three for the heavy holes, and one for the light holes. Of note in the figures is the strength of the allowed $\Delta n=0$ transitions (HH1-CB1, HH2-CB2, and LH1-CB1) relative to the forbidden HH3-CB1 one. Also, the strain induced splitting of the heavy and light hole bands is clearly seen.

Excitons in these $InSb/Al_xIn_{1-x}Sb$ quantum wells are also seen up to room temperature. The advantage of this is that *InSb* based quantum wells are already attractive for high speed electronic devices due to a high intrinsic mobility and

narrow band gap. The existence of room temperature excitons increases the practicality of such devices. There are two reasons one can observe excitons in *InSb* at high temperatures despite their relatively small binding energy (0.5meV in bulk *InSb*). First is that electrons excited by optical absorption to excitons have no excess energy to create phonons, which could smear out the exciton spectrum. The second is that the coupling between the excitons and LO phonons in *InSb* is very weak [22] (~3meV) as compared to materials such as *GaAs* (10meV). Additionally, confinement in a quantum well leads to an increase in exciton binding energy over its bulk value (theoretically up to a factor of 4 in a truly two dimensional well with infinite barriers). Figure 5-11 shows the room temperature exciton spectrum for sample 595, which has a 9% aluminum concentration in the barrier. Also depicted are lower temperature exciton spectra, depicting temperature dependence.

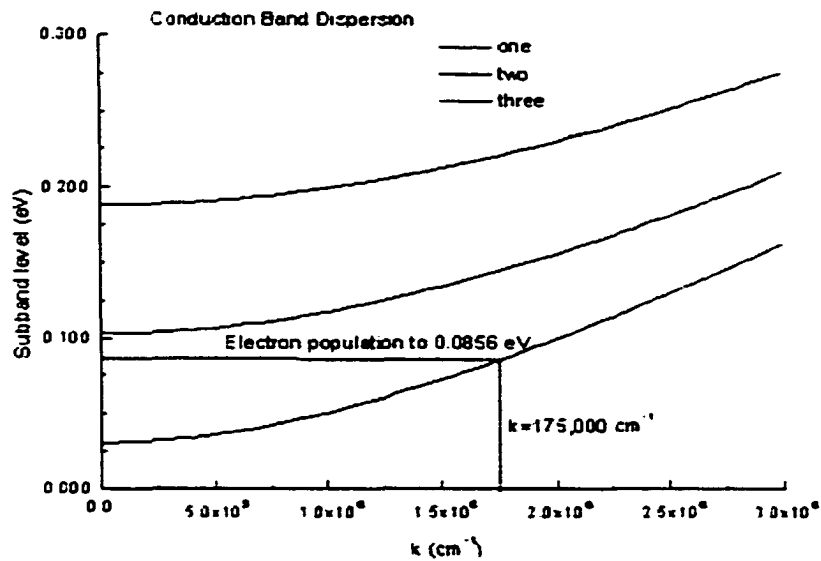


Figure 5-1 Conduction Subband Dispersion Curves

The value of k_F is found using $k_F = \sqrt{2m}$. The curves are numerically calculated.

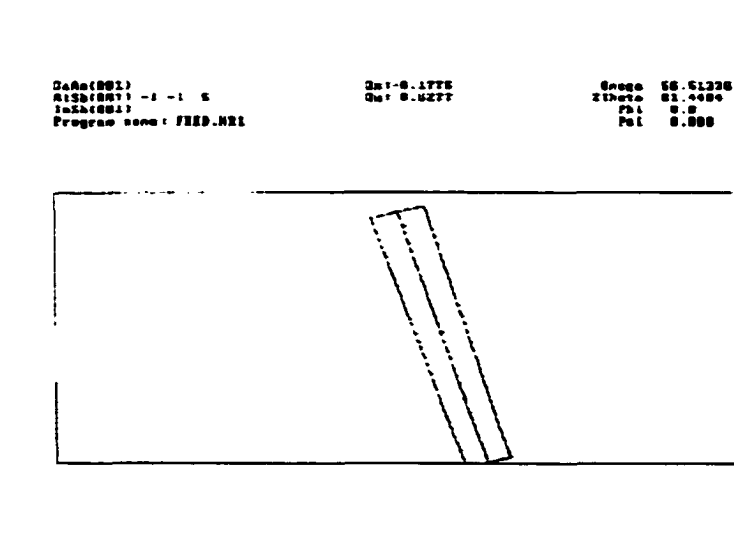


Figure 5-2 X-Ray Area Scan

Theoretical alignment of the $[-1 -1 5]$ reciprocal lattice point for unstrained *GaAs*, *AlSb*, and *InSb*.

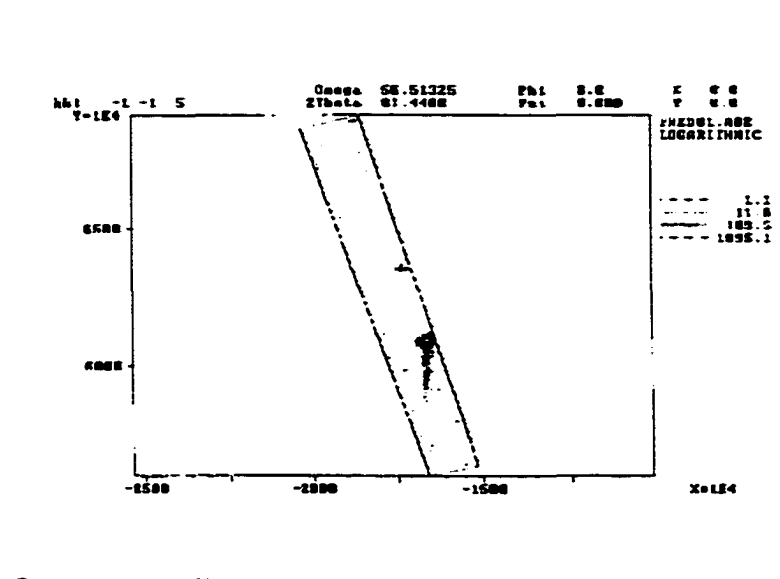


Figure 5-3 X-Ray Area Scan: 21.3% Aluminum

Measured area scan. The vertical tail downward is due to the lattice matched *InSb* quantum wells.

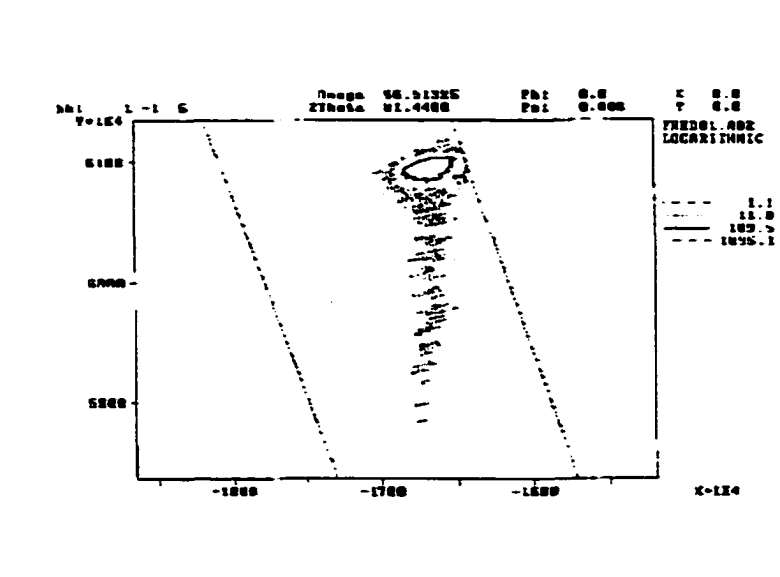


Figure 5-4 Enlargement of Figure 5-3

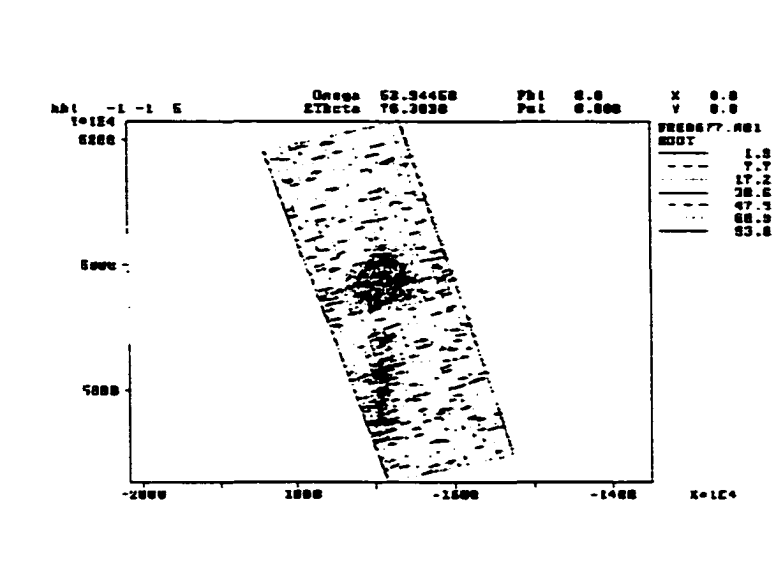


Figure 5-5 X-Ray Area Scan: 32.2% Aluminum

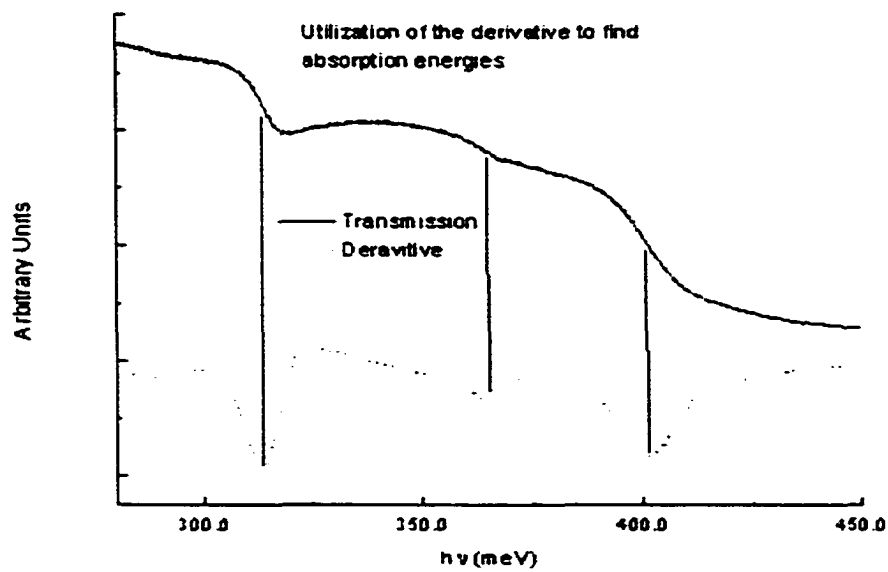


Figure 5-6 Transmission Spectrum and Derivative

The vertical lines highlight the enhancement of exciton transitions in the derivative of the spectrum.

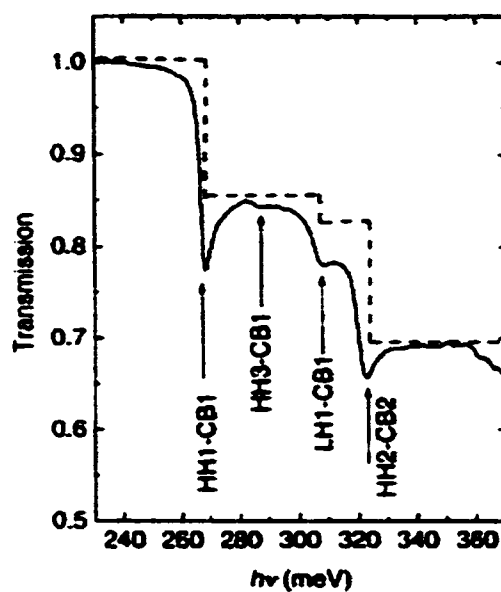


Figure 5-7 Transmission Spectrum of S595

The step-like structure is due to the 2D DOS. Note that the "forbidden" transitions are weaker than the $\Delta n=0$ transitions.

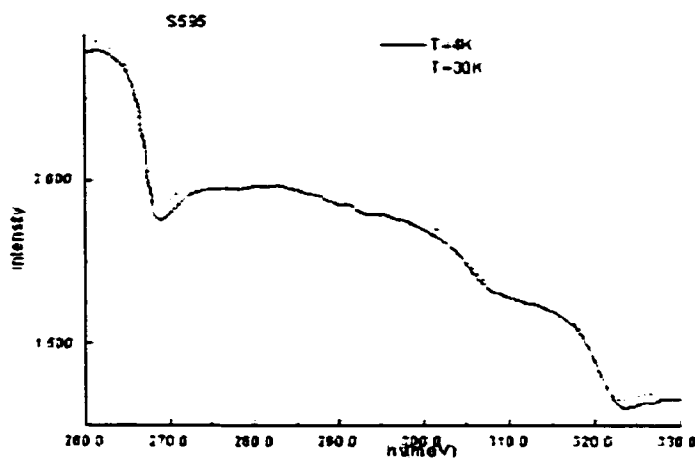


Figure 5-8 Raw Spectrum of S595

There is little difference between the spectra at different temperatures except when the interband transitions occur.

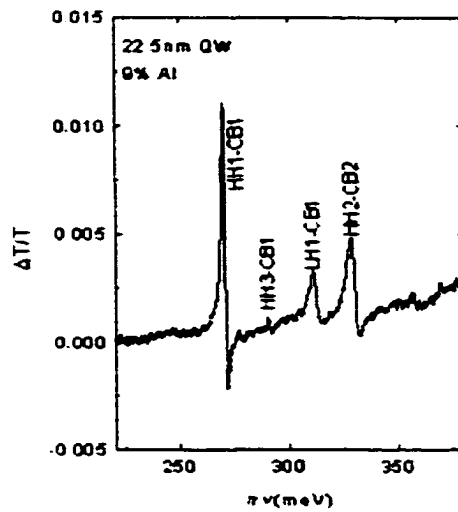


Figure 5-9 Difference Spectrum of S595

Spectrum of sample S595, highlighting the enhanced features of the difference spectrum.

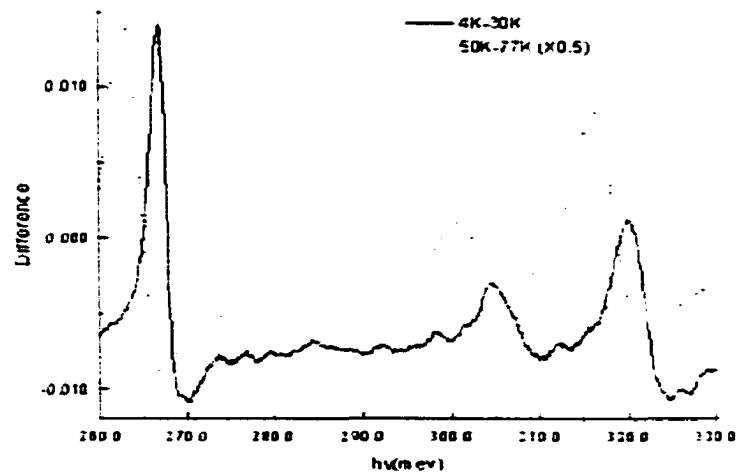


Figure 5-10 Temperature Dependent Broadening of Difference Spectra

The band gaps of *InSb* and *AlInSb* are more strongly dependent on temperature at higher temperatures. This is the reason that the higher temperature difference spectrum is broader, even though the temperature difference in each case is the same.

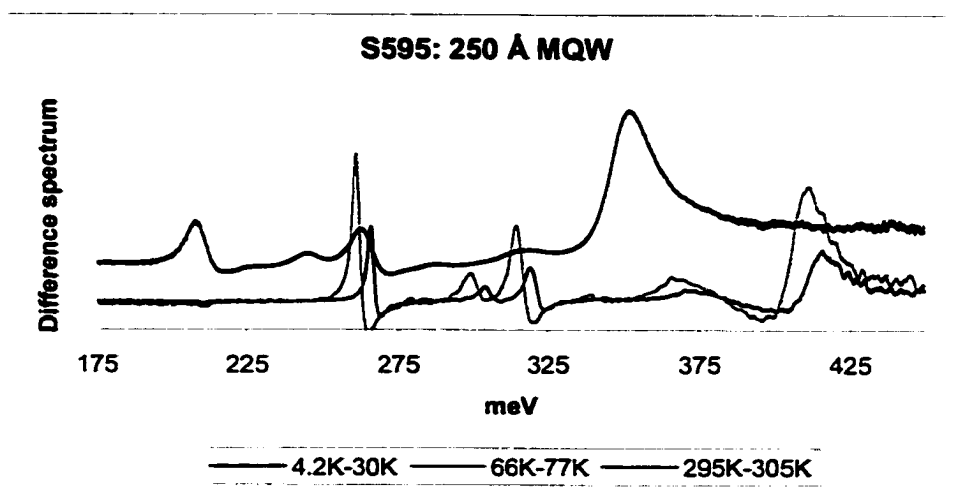


Figure 5-11 Various Temperature Exciton Spectra of S595

As expected, all features shift to lower temperatures with increasing temperatures. Of note is that the exciton transitions are still observed at room temperature in *InSb*.

Chapter 6: Dependence of the $\text{Al}_x\text{In}_{(1-x)}\text{Sb}$ Band Gap on Aluminum Concentration and Temperature

6.0 Introduction

The physical properties of $\text{InSb}/\text{Al}_x\text{In}_{1-x}\text{Sb}$ quantum wells depend on aluminum concentration as well as temperature. $\text{Al}_x\text{In}_{1-x}\text{Sb}$, used as barrier layers for the quantum well system, has a band gap range from 0.237eV (at $x=0$) to 2.38eV (at $x=1$). For a given well width, the confinement of the electrons and holes in the quantum well can be tuned by changing the aluminum concentration, x . The band gaps of both the well and the alloy layers are temperature dependent. As a result, excitonic transition energies depend both on temperature and alloy composition, in addition to the geometric parameters of the quantum well system (such as thickness of InSb well layers). Previously, Agaev et. al. [23] and Isomura et. al. [24] carried out studies of the alloy band gap as a function of Al concentration at 300K. However, these are very limited data in the lower aluminum concentration ranges (say, $x<20\%$), which are of great interest for device applications. Thus, a detailed understanding of the band gap dependence of the $\text{Al}_x\text{In}_{(1-x)}\text{Sb}$ alloy on temperature and aluminum concentration is essential, which was the prime motivation for this portion of the research. In this chapter, a detailed study of the InSb and alloy band gaps as a function of aluminum concentration and temperature is presented. The studied temperature range is from 4.2K to 300K and concentration ranges from 0 to 0.25. This study forms the basis for the research described in Chapters 7, 8, and 9.

6.1 Samples

All samples were epitaxial layers grown by MBE on *GaAs* substrates. Sample structure consists of a nominal 1 micron *AlSb* buffer layer, 2 micron alloy layer, and 2 microns of *InSb* as a capping layer to prevent oxidation of the alloy (see Figure 6-1). In all samples, the alloy is fully relaxed - as is the capping layer in all samples other than that with $x=0.05$. Verification of complete relaxation of the epitaxial layer is determined via high-resolution x-ray diffraction (HRXD) area scan at the (511) point in reciprocal space with the MRD system at 300K as discussed in Chapter 5. When unstrained, the *InSb* cap layer serves as a reference point for calibrating the x-ray system to determine alloy lattice constants (the *GaAs* substrate peak would need to be used as a reference when the cap layer is unstrained). The lattice constant of the alloy is assumed to depend on aluminum concentration through Vegard's law. By measuring the angular separation of the {004} peaks between *InSb* and $Al_xIn_{1-x}Sb$ on a rocking curve, one can compute the alloy lattice constant. This is done by applying the Bragg condition, $\lambda = d \sin \omega$ where ω is the (calibrated) angular position of the alloy peak. This is discussed in detail elsewhere [18]. One can then calculate the aluminum concentration from the alloy lattice constant.

6.2 Results

6.2.1 Concentration Dependence

Six samples with aluminum concentrations of 5% through 30% were studied. For each sample, a series of HRXD rocking curves were taken at different sample orientations and the aluminum concentration was determined from averaging the

value at each orientation. Figure 6-2 shows one such curve. A series of single beam spectra were then taken at different temperatures for each sample. Transmission spectra relative to a *GaAs* substrate clearly showed the alloy absorption edges (marked with arrows for the three samples shown in Figure 6-3), the position of which was determined by the high energy point of steepest slope, as discussed in Chapter 5.

A plot of the measured energy gap at 4.2K versus the shift in lattice constant ($\Delta a = a_{\text{alloy}} - a_{\text{InSb}}$) in Figure 6-4 [55] shows a linear relationship, given by:

$$E_{g_{\text{alloy}}} = E_{g_{\text{InSb}}} + E'_g \Delta a,$$

Equation 6-1

where E'_g (eV / Å) is the measured slope. Table 6-1 gives the values for *InSb* gap and E'_g at 4.2K, 77K, and 300K. Application of Vegard's law:

$$a_{\text{alloy}} = a_{\text{InSb}}(1 - x) + a_{\text{AlSb}}x$$

Equation 6-2

yields $\Delta a = 0.343x$ (where at 300K, $a_{\text{InSb}} = 6.479 \text{ Å}$ and $a_{\text{AlSb}} = 6.136 \text{ Å}$).

Combining this with Equation 6-1 enables one to calculate the aluminum concentration from the band gap absorption edge of the alloy:

$$E_g(\text{alloy}) = E_g(\text{InSb}) + E'_g(0.343)x$$

Equation 6-3

For concentrations lower than 25%, one can read the aluminum concentration on the top axis of Figure 6-4 for a measured absorption edge. For higher concentrations, the transitions move beyond the mid-IR region and out of the available range of the spectrometer. Additionally, this model would fail for very high aluminum concentrations as the transitions become indirect since AlSb is an indirect gap semiconductor.

This data compares favorably to that of Agaev and Bekmedova done at 300K. In comparison with the work of Isomura *et al.*, these values for alloy band gaps are higher. The consistency between the 300K measurements of the *InSb* energy gap - and those of Isomura, et. al. - indicates that the high concentration difference is not due to the different measurement techniques (transmission versus electroreflectance). Additionally, agreement on the extrapolated value for the AlSb direct gap indicates that this disagreement may come from determination of the aluminum concentration rather than from band gap measurements.

6.2.2 Temperature Dependence

A complete study of alloy band gap as a function of temperature was also performed.

As shown in Figure 6-5, the band gap energy increases as temperature is reduced. At higher temperatures, the dependence is linear in nature. As temperature is decreased, the change in band gap energy saturates. This variation of energy gap with temperature - linear at high temperature and quadratic for lower temperatures - has been observed for many materials. The empirical relation:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{\beta + T}$$

Equation 6-4

first used by Varshni [25] describes this behavior well for a large variety of semiconductors. Generally, α and β are used as fitting parameters and their values vary with material system. Even for measurements on the same materials, however, there are large disagreements [26] [27]. Not only have different values been determined for samples grown by different methods and over different temperature ranges, but a dependence on measurement technique has also been noted [26] [28].

Many authors have attempted to invest these parameters with physical meaning. The evaluated values for β are usually near the Debye temperature of the materials being studied, so it has been assumed that they are related. While it is easy to relate α as the infinite temperature gap entropy [29], it is generally only interpreted as a fitting parameter [28] [30]. In some work, β is fixed as the Debye temperature and $E_g(0)$ is determined by fitting the curve [28] [30]. In the latter study, varying β by as much as 50% had minimal effect (on the order of 2meV) on the final value of $E_g(0)$.

The data in Figure 6-5 for *InSb* and each of the alloys generally agrees with the work of Littler and Seiler [31] in that the gap temperature dependence fits the Varshni formula. However, there is a large disparity in the values of α and β . In the present work, β is close to the Debye temperature of *InSb* (203K), as is generally found in

other semiconductors. Additionally, the 300K value of $\frac{dE_g}{dT}$ is consistent with published values [12]. This is not the case with the study done by Littler and Seiler. Fits to the data in this work are represented by the solid lines in Figure 6-5. The fit using the α and β found by Littler and Seiler is shown in the top plot with a dashed line. As can be seen, their values provide a poor fit to this data at higher temperatures. Table 6-2 lists α , β , and $\frac{dE_g}{dT}$ for all samples.

6.3 Discussion

The Debye temperature is frequently used to divide the high temperature from the low temperature regime [25]. As such, it can be used as a measure of where the energy gap should (roughly) end its quadratic behavior and tend towards linearity. As the parameter β is so strongly determined by this division and is frequently close to the Debye temperature, it would be convenient to compare the two over a range of aluminum concentrations. For most alloys, however, the Debye temperature is not known. Some authors have attempted to find a relationship with concentration. Sanchez-Almazan, et. al. assumed a linear variation with zinc content of the Debye temperature in their work on $Cd_{(1-x)}Zn_xTe$ so that they could fit $E_g(0)$. Lunz, et. al. [32] expressed both α and β as functions of concentration, though they had to introduce a new parameter in their quadratic expression for β . For the $Al_xIn_{(1-x)}Sb$ alloy system, a linear relationship for β was not found using the Debye temperatures of 203K and 292K for $InSb$ and $AlSb$, respectively.

6.4 Conclusions

This study of the dependence on temperature of *InSb* and its alloys has provided a better understanding of the excitonic spectra observed in the *InSb* / $Al_xIn_{1-x}Sb$ quantum well systems. Results are in general agreement with related studies conducted by others on this material system and expand on the limited data for lower aluminum concentrations. Perhaps the most frequently used result in the remainder of this research is the ability to determine alloy aluminum concentration from the position of the measured absorption edge (Equation 6-3). Additionally, these results are the basis for further studies pertaining to band alignment at *InSb* / $Al_xIn_{1-x}Sb$ heterojunctions, and the effects of strain and doping in quantum wells.

2 micron InSb
2 micron alloy
1 micron AlSb buffer
GaAs Substrate

Figure 6-1 Diagram of Epitaxial Layers

A series of samples were grown with different *Al* concentrations in the alloy layer. The top layer of *InSb* protects the alloy from oxidation.

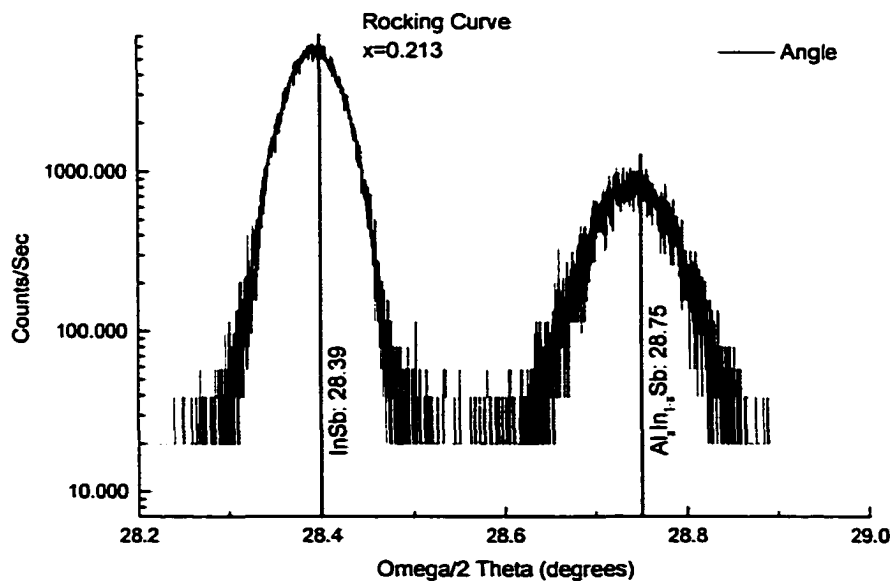


Figure 6-2 HRXD Rocking Curve

The rocking curve gives angular separation between the scattering peaks due to *InSb* and *AlInSb* (or *GaAs*). This helps determine the alloy lattice spacing, from which one can determine the aluminum concentration via Vegard's Law.

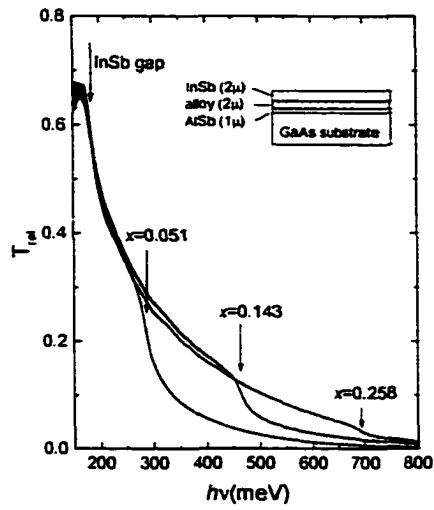


Figure 6-3 Alloy Absorption Edges

The absorption edge of the alloy shifts to higher energy with increasing aluminum concentration. This is expected due to the smaller lattice constant of the alloy.

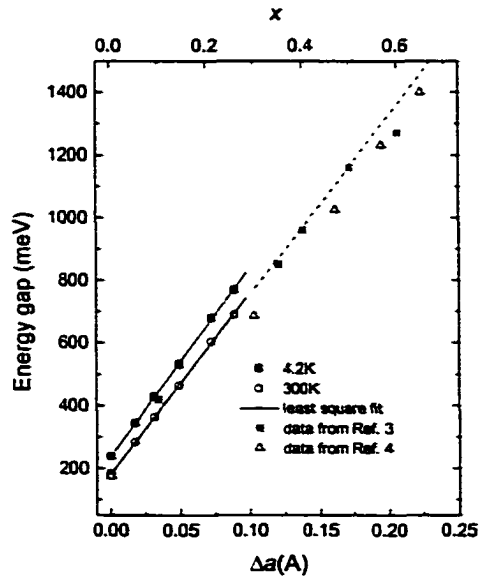


Figure 6-4 Energy Gap at 4.2K Versus Alloy Lattice Constant

A direct relationship between the change in lattice constant and aluminum concentration [55].

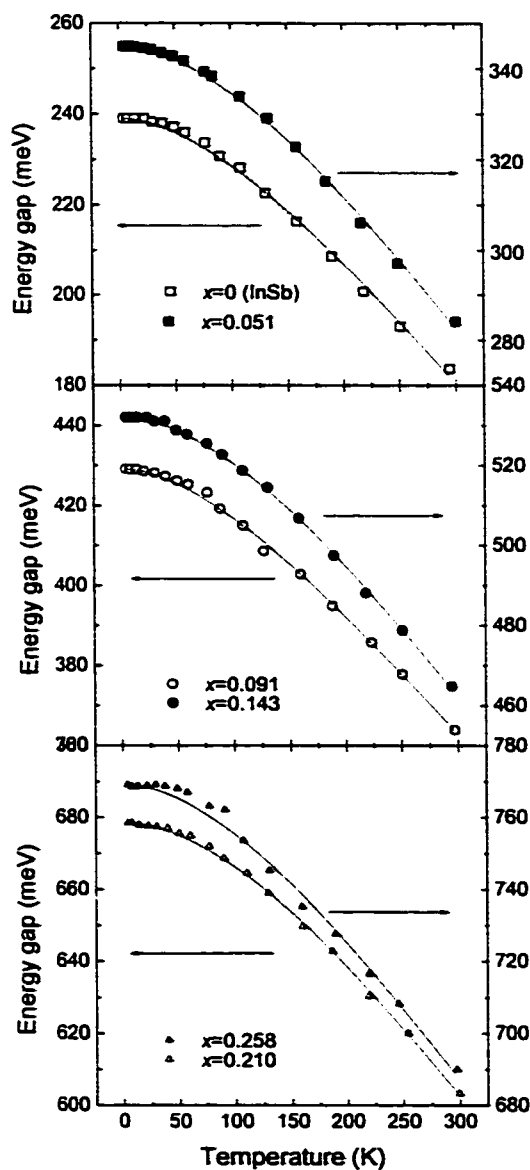


Figure 6-5 Alloy Band Gap Versus Temperature

The fit using the α and β found by Littler and Seiler [31] is shown in the top plot with a dashed line. The fits to the current data yield results listed in Table 6-2.

Table 6-1 Energy and Shift in Lattice Constant with Aluminum Concentration

Temperature (K)	$E_g(\text{InSb})$ (eV)	E'_g (eV / Å)
4.2	0.240±0.002	6.01±0.03
77	0.234±0.002	6.01±0.03
300	0.183±0.002	5.76±0.03

Table 6-2 Concentration, $\alpha(\text{meV} / K)$, $\beta(K)$, and $\frac{dE_g}{dT}(\text{meV} / K)$

Concentration (x)	$\alpha(\text{meV} / K)$	$\beta(K)$	$\frac{dE_g}{dT}(\text{meV} / K)$
0 (Littler and Seiler)	0.6	500	-0.366
0	0.35	236	-0.282
0.051	0.44	331	-0.317
0.091	0.37	196	-0.309
0.143	0.48	315	-0.353
0.210	0.53	326	-0.385
0.258	0.53	275	-0.405

Chapter 7: Band Offset

7.0 Overview and Statement of Results

Band offset is defined as the potential discontinuity of the valence or conduction band at a semiconductor heterojunction [33], ΔE_{cb} and ΔE_{hh} for the conduction and heavy hole bands, respectively. Defining Q_c as the ratio of the conduction band offset to the difference in band gaps of the barrier and well materials yields:

$$\Delta E_{cb} = Q_c \Delta E_g$$

Equation 7-1

and

$$\Delta E_{hh} = (1 - Q_c) \Delta E_g.$$

Equation 7-2

Q_c represents the partitioning of the band gap difference between the conduction and heavy hole bands. Figure 7-1 depicts each of these quantities for a simple square well system.

The determination of the band offset of quantum well structures is important for device design considerations as it determines the depth of the conduction and valence band wells and therefore the number of allowed subbands in each. Knowledge of the band offset is also required for the theoretical modeling of band structure. This series of experiments has yielded the value of $Q_c=0.62\pm0.04$ for the band offset of the

InSb / $Al_xIn_{1-x}Sb$ system. This is independent of the aluminum concentration, which ranged between $x=0.02-0.15$, indicating a lack of dependence on strain. This strain independence is supported by the consistency of results from experiments on both well strained and barrier strained samples.

Experiments were carried out on a number of samples with parabolic quantum wells. Figure 7-2 and Figure 7-3 present the differential transmission spectra of 500Å and 1000Å parabolic MQW's, respectively. Both samples have nominal aluminum concentrations of 9% and are well strained. In the figures, interband transition energies are labeled by $HHn(LHn)-CBm$ for transitions between the heavy(light) hole and conduction subbands, where n and m are indices of the valence subband (heavy hole or light hole) and the conduction subband, respectively. Selection of transition energies are via determination of the high energy inflection point, as discussed in Chapter 5, and are marked with solid lines in the figures. The reason for using this method for selecting the transition energies is the strong temperature dependence of the *InSb* band gap, so that the differential transmission spectra are essentially equivalent to the derivative of the corresponding transmission spectra. The utilization of a difference spectrum enhances structures corresponding to excitons and their continuum. Due to the excitonic features of the absorption spectra, onset, more commonly identified in transmission and absorption spectra, occurs at the peak of the transition in difference spectra. Of note in both figures is the occurrence of forbidden $\Delta n = 2$ transitions. From these, one can extract valence and conduction subband energy spacing, as discussed in detail later. Intersubband spacing between the n^{th} and

m^{th} subbands is represented by ΔCB_{nm} for electrons, ΔHH_{nm} for heavy holes, and ΔLH_{nm} for light holes, and - as will be shown - is essential for determining band offset. An additional set of square well samples was studied in which the “forbidden” HH3-CB1 transition was also observed. Determination of band offset from these samples is in good agreement with that from the parabolic samples. All samples were nominally undoped.

Experimental techniques other than optical spectroscopy to determine band offset belong either in the category of electron spectroscopy or electrical measurements. X-ray photoelectron spectroscopy (XPS) has been used to determine core level binding energies relative to valence band edges in two materials. This has been primarily done in unstrained heterojunctions with the largest source of error coming from determination of the valence band edge in the spectra. Use in strained systems requires accurate deformation potentials between core levels (both in bulk materials and strained layers) and valence band edges in bulk materials.

One type of electrical measurement which has been used is thermionic emission. Band offsets are deduced from the dependence of the current density on temperature and barrier heights across an interface. Another method is capacitance-voltage measurements across a heterojunction. This technique is based on conservation of carriers and how they are distributed and was used by Kroemer et. al. in 1980 to determine $Q_c=0.66$ for the *GaAs* system [34], which is close to the currently accepted value. The difference with the value of $Q_c=0.85$, which was accepted at the time (and

will be discussed below), was explained as due to compositional grading. In fact, both XPS [35] and C-V measurements were used and supported the earlier findings of Dingle, et. al., which highlights the need for care regardless of the technique used.

7.1 Theory/ Samples /Method of Analysis

7.1.1 Theory

While conceptually straightforward, band offset has historically been a difficult parameter to determine, both in theory and in experiment. The early work by Dingle [36] on $GaAs/Al_xGa_{1-x}As$ square quantum wells led to an erroneous result of $Q_c=0.85$ for that system. The difficulty with square quantum wells is that the lowest subbands depend very weakly on the band offset and can be reasonably modeled by an infinite barrier. This was done by Dingle for the conduction and valence subbands with good results for observed exciton transition energies. Subbands in narrow square wells are more sensitive to the value of Q_c due to the $\sim \frac{1}{L_z}$ dependence of subband energy. However, there are fewer confined states in narrow wells resulting in fewer exciton transitions. Additionally, forbidden transitions ($\Delta n \neq 0$) in square quantum wells are generally weak. As a result, band offset cannot be reliably extracted from data on square quantum wells.

This series of experiments follows the method used by Miller et. al. [37] [38] in their study of $GaAs/Al_xGa_{1-x}As$ that resulted in a value of $Q_c \approx 0.57$ - close to the currently accepted value of $Q_c \approx 0.6$. $InSb/Al_xIn_{1-x}Sb$ multiple quantum wells with

parabolically graded barriers are used. There are multiple purposes for this potential shape. First, the subband energies are equally spaced (in the limit of an infinite well) at

$$E_n = (n - \frac{1}{2})\hbar\omega$$

Equation 7-3,

$n=0,1, 2, 3$, etc., where $\omega = \sqrt{\frac{k}{m^*}}$. As the potential is of the form

$$V = \frac{1}{2}kz^2,$$

Equation 7-4

a well of width L_z would have a conduction band offset of

$$V = \Delta E_{cb} = Q_c \Delta E_g = \frac{1}{2}kz^2 \Big|_{z=\frac{L_z}{2}}.$$

Equation 7-5

The resulting $k = \frac{8Q_c \Delta E_g}{L_z^2}$, yields

$$E_{cb}^n = (n - \frac{1}{2}) \frac{2\hbar}{L_z} \left(\frac{2Q_c \Delta E_g}{m_e^*} \right)^{\frac{1}{2}}$$

Equation 7-6

for the n^{th} conduction subband energy. Likewise, one gets

$$E_{hh}^n = (n - \frac{1}{2}) \frac{2\hbar}{L_z} \left(\frac{2(1 - Q_c) \Delta E_g}{m_{hh}^*} \right)^{\frac{1}{2}}$$

Equation 7-7

for the n^{th} heavy hole subband. Intersubband spacing is related to the above equation

by $\Delta CB_{nm} = E_{cb}^n - E_{cb}^m$ with a similar equation for the heavy hole subbands,

$\Delta HH_{nm} = E_{hh}^n - E_{hh}^m$. The ratio of these quantities is given by

$$\frac{\Delta CB_{nm}}{\Delta HH_{nm}} = \left(\frac{Q_c}{1 - Q_c} \frac{m_c^*}{m_{hh}^*} \right)^{\frac{1}{2}}$$

Equation 7-8

which explicitly depends on the conduction band offset.

The second purpose for parabolic wells is the occurrence of the strong $\Delta n = 2$ transition. The reason these transitions are so strong is that low index states are more tightly confined than higher states due to the differing well widths for each state. Therefore, different index states do not experience the same confining potential or well width. Additionally, the different curvature of the conduction and valence bands, combined with the strong non-parabolicity of the conduction band, ensure that different index states are non-orthogonal. Another advantage these wells have over square quantum wells is due to the strained nature of these heterostructures. This method of extraction of band offset from spectra depends on multiple $\Delta n = 2$ and $\Delta n = 0$ transitions. For a square well, a large number of transitions requires that either the barrier be high or that the wells be wide, both of which lead to misfit

dislocation. Due to the design of the parabolic quantum wells, this can be avoided while still ensuring sufficient transitions.

7.1.2 Samples

The idealized potential profile of a finite parabolic quantum well is shown in Figure 7-4. The splitting of the heavy and light hole valence bands is due to strain, and will be examined in detail in the next chapter. As with all other samples, these were grown by MBE. To achieve wells with a smooth parabolic potential profile would require a degree of control over the fluxes of the source materials that is impractical at present. As was done by Miller et. al.[37], the parabolic profile was modeled by dividing the wells into segments of thickness $\frac{L_z}{20}$, where L_z is the well thickness.

Each segment contains an $Al_xIn_{1-x}Sb$ layer and an $InSb$ layer and they are centered on an $InSb$ layer. Keeping the aluminum concentration in the layers identical to the barrier concentration, the desired profile is achieved by varying the thickness of each layer quadratically with increasing distance from the center of the well such that the alloy gets thicker and the $InSb$ gets thinner. The thickness of the N^{th} layers as counted from the center of the well are given by

$$\delta_{Al_xIn_{1-x}Sb}^N = \left(\frac{N-0.5}{10} \right)^2 \frac{L_z}{20}$$

Equation 7-9

and

$$\delta_{InSb}^N = \frac{L_z}{20} - \frac{N^2 - 0.5^2}{100} \frac{L_z}{20}.$$

Equation 7-10

These narrow alternating layers ensure that excitons in *InSb* experience an effective parabolic confining potential due to their 600 Å Bohr radius being on the order of the well width.

The choice of well width and aluminum concentration for these samples was dictated by the desire to study the effects of strain and concentration on band offset, as well as any dependence on well width. Additionally, the wells had to be wide and deep enough to hold enough states so that band offset could be determined via the method discussed below. Balancing well width and concentration versus layer critical thickness set the criteria for well strained and barrier strained samples. For this set of samples, well widths were 400 Å, 500 Å, and 1000 Å with 25 wells. Barrier widths were 300 Å for barrier strained samples and 500 Å for all others. Considering the large Bohr radius for excitons in *InSb* (on the order of 600Å), these widths are below the regime for bulk excitons. A diagram of a 1000 Å MQW is given in Figure 4-3, Chapter 4. Aluminum concentration in the samples varied from x=0.02-0.15. For those with x>0.09, the *InSb* layers were partially relaxed, as verified by x-ray analysis. Barrier strained samples were grown by including a 2 micron *InSb* layer between the buffer and quantum wells so that the $Al_xIn_{(1-x)}Sb$ layers would be lattice matched to the *InSb* layers. Table 7-1 tabulates these parameters for the parabolic quantum wells.

7.1.3 Method of analysis

From direct observation of these spectra one can determine the exciton transition energies, HHn-CBm. Such transitions between the first and third conduction and heavy hole subbands are depicted in Figure 7-5. From taking the difference between two of these transitions one can determine the spacing between two of the subbands. For example, the energy difference between the first and third conduction subbands - ΔCB_{13} - can be determined by subtracting the HH3-CB1 energy from the HH3-CB3 energy. Alternatively, one can subtract HH1-CB1 from HH1-CB3 to get the spacing. This example highlights the need for the $\Delta n = 2$ transitions mentioned earlier. The hole subband spacing is determined in a similar manner. The experimental number from which the conduction band offset is determined is the ratio $\frac{\Delta CB_{nm}}{\Delta HH_{nm}}$.

The earlier discussion on theory that resulted in $\frac{\Delta CB_{nm}}{\Delta HH_{nm}} = \left(\frac{Q_c}{1-Q_c} \frac{m_e^*}{m_{hh}^*} \right)^{\frac{1}{2}}$ was based on infinite wells with a continuously graded interface. These conditions being unrealistic, combined with the non-parabolicity of the *InSb* band structure, mean that this equation cannot be used as is. Rather, $\frac{\Delta CB_{nm}}{\Delta HH_{nm}}$ is numerically calculated [39] as a function of the offset, using a four-band model [40], with Q_c as the only free parameter. The *InSb* conduction band non-parabolicity and layered structure of the quantum wells are included in the calculations (the heavy hole band is approximated as parabolic). Also necessary to the calculations are the band gaps of the layers of

InSb and $Al_xIn_{1-x}Sb$. The latter are measured via FTIR and aluminum concentration is verified by the method discussed in the previous chapter. The effect of strain on the well band gap is also included, though its effect should be minimal due to measuring energy differences, as should that of the exciton binding energy. The assignment for the value for Q_c comes from the best agreement between the experimentally determined ratio for subband spacing and the numerically calculated curve for $\frac{\Delta CB_{nm}}{\Delta HH_{nm}}$. Of final note is the importance of the effective mass ratio $\frac{m_e^*}{m_{hh}^*}$ used in the calculations. As discussed by Rössler [41], cyclotron hole mass can only be used instead of the dispersion mass when there is minimal warping of the surfaces of constant energy. As conduction band warping is insignificant, the *InSb* cyclotron effective mass [12] for the electron, $m_e^* = (0.0139 \pm 0.0001)m_0$, and the Luttinger effective mass for $m_{hh}^* = (0.25 \pm 0.01)m_0$ (where m_0 is the electron rest mass) in are used in these calculations.

7.2 Results/Comparison with Calculation

7.2.1 Fully strained

For the first set of parabolic quantum wells studied, the *InSb* layers are under compressive strain and lattice matched to the $Al_xIn_{1-x}Sb$ alloy. This lifts the degeneracy of the heavy and light holes, as depicted in Figure 7-4 and seen in the spectra of S578 and S555 (Figure 7-2 and Figure 7-3). For both samples, the $\Delta n = 2$

transitions yields the $\frac{\Delta CB_{13}}{\Delta HH_{13}}$, as is necessary for the determination of Q_c . Figure 7-6

is a plot of this ratio numerically calculated as a function of conduction band offset for a 1000 Å sample (S555). (The solid line labeled as 1000 Å in the figure.) The experimentally determined ratio is represented by the cross hatched region. The range of values is a result of uncertainty in marking the transition positions. From the intersection of the 1000 Å line and the cross-hatched region, one gets a value of $Q_c=0.63\pm0.03$ for this sample. The last column of Table 7-1 lists the determined offsets with errors for each of the parabolic samples. The average conduction band offset (and error) for this set of samples is $Q_c=0.62\pm0.04$. There is also an uncertainty in the well width of about $\pm 5\%$. As can be seen from the calculated 1050 Å line, this contributes to the uncertainty in Q_c to smaller degree than the uncertainty in $\frac{\Delta CB_{13}}{\Delta HH_{13}}$. The dashed line in Figure 7-6 is calculated based upon Equation 7-1.

The shift seen in the 1000 Å and 1050 Å lines are due to *InSb*'s non-parabolic band structure and finite barrier height.

Since both the ΔCB_{13} and ΔHH_{13} subband spacing can be found in two ways (HH3-CB3 minus HH3-CB1 or HH1-CB3 minus HH1-CB1 for ΔCB_{13} ; and HH3-CB3 minus HH1-CB3 or HH3-CB1 minus HH1-CB1 for ΔHH_{13}), peak assignments due to numerical computation can be alternatively verified. For the 500 Å sample (S578), this is unnecessary due to the clear separation between transition peaks. For the 1000 Å samples, this verification is especially advantageous due to many more transitions,

which are close in energy. For the two fully strained samples with $x > 0.06$ and a width of 1000 Å samples (S555 and S634), the ratio $\frac{\Delta CB_{24}}{\Delta HH_{24}}$ is also attainable as conditions allow the occurrence of the fourth subbands in the conduction and heavy hole bands. This provided an alternate means of determining the offset ratio with results that were consistent with the $\frac{\Delta CB_{13}}{\Delta HH_{13}}$ ratio.

7.2.2 Partially relaxed

The next set of samples studied (S580, S575, S568 and S579) were determined to be partially relaxed by mapping the {115} reciprocal space lattice point in an area scan via HRXD as discussed in Chapter 5. The percent relaxation listed in Table 7-1 was determined by taking dual rocking curves as detailed in the x-ray diffractometer user guide [42]. Since the energies of the lowest index ($n=1$) states are most sensitive to the position of the bottom of the well, additional verification of the degree of relaxation comes from comparison of the measured HH1-CB1 transition energies with calculations that account for the degree of strain. This is because it is the *InSb* well material that accommodates relaxation via misfit dislocations, altering the well gap from the fully strained condition. The $Al_xIn_{1-x}Sb$ alloy remains strain free, enabling one to still determine aluminum concentration from the position of E_g^{alloy} . The percent relaxation is defined as

$$R\% = \left(\frac{a_{\text{measured}} - a_{\text{Al}_x\text{In}_{1-x}\text{Sb}}}{a_{\text{InSb}} - a_{\text{Al}_x\text{In}_{1-x}\text{Sb}}} \right) 100 .$$

Equation 7-11

where a_{measured} is the lattice constant of the partially relaxed InSb layers and a_{InSb} is the bulk InSb lattice constant.

Figure 7-7 is the difference spectrum of S580, which has a 15% relaxed well. In comparison to S578 (Figure 7-2), line widths show little deterioration, despite mismatch dislocations. Differences in transition energies are accounted for by strain effects and different barrier heights. As with the fully strained samples discussed above, offset was determined for these samples by the intersection of the measured $\frac{\Delta CB_{13}}{\Delta HH_{13}}$ range with the calculated curve (taking into consideration the partial strain relaxation). The resulting average is consistent with the fully strained average at $Q_c = 0.64 \pm 0.04$.

7.2.3 Barrier strained

Two final samples (S637 and S638) were grown in which the $\text{Al}_x\text{In}_{1-x}\text{Sb}$ layers were strained rather than the InSb . The purpose of these samples was to determine what, if any, effect strain has on Q_c and will be discussed more fully in the next section. To prevent lattice relaxation, thin barriers and low aluminum concentrations were chosen in addition to the thick InSb layer between the buffer layer and barrier. Despite the thin barriers, adjacent quantum wells can still be considered uncoupled as calculations

show that - for $x=0.06$ and $L_z=300 \text{ \AA}$ - the CB3 wavefunction is predominantly confined to the well. A simple calculation based on transmission probability assuming $L=300 \text{ \AA}$ and $V_0=76\text{meV}$ (corresponding to $Q_c=.62$ and $x=.06$) and $E=46\text{meV}$ (for CB3 in parabolic approx.) yields $T(E)=0.0072$.

The absorption spectrum for the $x=0.057$ sample (S637) is shown in Figure 7-8. An absorption peak at 237meV is seen in this sample due to the thick *InSb* layer inserted prior to the quantum wells. The red shift in transition energies as compared to S557 in Figure 7-9 (which has the same well width and aluminum concentration) is due to the lack of strain in the *InSb* layers. The heavy and light holes are again non-degenerate. In this case, degeneracy is lifted only due to the confinement of the quantum wells. The average band offset is 0.58 ± 0.03 for these samples. The lower Q_c for these samples can be explained in part by the fact that one cannot accurately determine the aluminum concentration as was done for the other samples due to the barrier alloy being under tensile strain. The assigned values for concentration for S637 and S638 assume the barriers to be strain free. The actual values should be larger due to the strain. The assigned values are what go into the numerical calculations and would therefore affect the resulting value of Q_c . Despite this, the determined values of Q_c for the barrier strained samples are consistent with those found for the other samples, indicating that any effect due to strain on Q_c is minimal.

7.3 Discussion of Strain, x , Q_{lh} , and temperature

The effects of strain and aluminum concentration, x , must be considered when determining the band offset for the $InSb / Al_xIn_{1-x}Sb$ material system. Figure 7-10 plots the determined Q_c 's for the completely strained parabolic wells as a function of aluminum concentration. The lack of measurable variation of Q_c with increasing x indicates that either band offset is independent of concentration and strain over this range of x , or that their effects cancel out. The answer comes in part from comparing the partially strained samples to the fully strained samples. For the latter group, the amount of strain in the wells is proportional to the aluminum concentration. Therefore, a sample that is fully strained with $x=0.07$ is under the same strain as a 50% relaxed sample with $x=0.14$. The consistent value of Q_c for samples which have similar strain and different aluminum concentrations (e.g. S579 ($x=0.1449$, 30% relaxed) with S607 ($x=0.112$, fully strained)) and of S568 ($x=0.1438$, 50% relaxed) with S634 ($x=0.0667$, fully strained) strongly suggests that band offset ratio for the $InSb / Al_xIn_{1-x}Sb$ is independent of aluminum concentration over the range studied. This of course means that the actual offset would be linear in concentration, as the alloy band gap was found to be in the last chapter. This is similar to the apparent linear dependence in x found for the offset in the direct gap range for the $GaAs / Al_xGa_{1-x}As$ system, which is unstrained [33] [43].

For light holes, one must consider how to define band offset. If it is defined in terms of the heavy hole band gap difference - $Q_{lh} = \frac{\Delta E_{lh}}{\Delta E_g}$ where ΔE_{lh} is shown in Figure

7-1 - then it's value must depend on strain as that is what lifts the degeneracy of the heavy and light hole bands. To define the light hole band offset in terms of the light hole band gap, the effects of strain must be considered. Both the heavy and light hole band gaps are shifted by strain. Assuming strain to be linear with aluminum concentration, the energy shifts take the form:

$$E_{\pm} = [(2 - 2\frac{C_{12}}{C_{11}})a \pm (1 - 2\frac{C_{12}}{C_{11}})b]\varepsilon_{\parallel},$$

Equation 7-12

where the C_{ij} are elastic constants, a and b are the hydrostatic and shear deformation potentials, and $\varepsilon_{\parallel}$ is the in plane strain given by

$$\varepsilon_{\parallel} = \frac{a_{\text{alloy}} - a_{\text{InSb}}}{a_{\text{InSb}}} x$$

Equation 7-13

The plus corresponds to the light hole shift and the minus to the heavy hole shift.

Taking the strain induced splitting of valence band energies into account, one can define the light hole band offset in terms of the light hole band gap:

$$Q_{lh} = \frac{\Delta E_{lh}}{\Delta E_g^{lh}} = \frac{(1 - Q_c)\Delta E_g - (E_+ - E_-)}{\Delta E_g - (E_+ - E_-)},$$

Equation 7-14

where $E_+ - E_-$ is the energy difference between the light and heavy hole bands. As seen above, Q_c is independent both of strain and aluminum concentration. As both ΔE_g and $E_+ - E_-$ are proportional to aluminum concentration, use of this definition for the light hole band offset means that Q_{lh} is independent of both strain and aluminum concentration. The data yield a value of $Q_{lh} \sim 0.24$ for the $InSb / Al_xIn_{1-x}Sb$ system.

The temperature dependence of band offset would also be useful to know as most device applications would likely be above the 77K. For both $InSb$ and its alloy, however, the strong temperature dependence of the band gap levels off below 77K. The variation in band gap for each is less than 10meV over that temperature range (Figure 6-5), which is too small to detect any variation in offset ratio. On the other hand, the exciton absorption peaks broaden significantly at higher temperatures, such that the uncertainty in determining location would yield any results meaningless.

7.4 Square well samples

While generally insufficient in and of themselves for the determination of band offset due to a lack of “forbidden” transitions, square quantum wells can be used under certain conditions. Nearly strain free systems, such as $GaAs / Al_xGa_{1-x}As$, allow wells to be designed that are both wide and deep. This ensures a large number of subbands in both the conduction and valence bands. Higher index subbands are most

sensitive to barrier height, which is set by the band offset, and can be useful in its determination.

The study of band offset using $InSb/Al_xIn_{1-x}Sb$ square quantum wells is more difficult as it is a strained system. Therefore well width must be balanced with barrier height (aluminum concentration) such that there are enough states available to determine band offset without exceeding the critical thickness of the well material. Additionally, strain effects must be taken into account as discussed earlier. For this portion of the band offset study, a series of three undoped square quantum well samples were grown, all with aluminum concentrations of ~9%. The wells were thin enough such that they were fully strained, yet wide enough to accommodate at least 2 conduction subbands and 3 valence subbands. Table 7-2 lists the parameters for these samples.

The difference spectrum in Figure 7-11 is of a 225 Å MQW (S589). Calculations using $Q_c=0.62$ predict 2 conduction subbands, 1 light hole state and 4 heavy hole subbands. There is only one light hole state due to its small mass and the strain induced reduction in its well depth. Clearly seen in the spectrum are the HH1-CB1, HH2-CB2 and LH1-CB1 transitions. Also seen, but much weaker, is the HH3-CB1 transition. The occurrence of this forbidden transition is due in part to the conduction band non-parabolicity, which reduces the orthogonality of these subbands.

Additionally, Dingle originally came up with his selection rules based on a single particle model in an infinite square quantum well. While these $\Delta n = 0$ transitions are

the strongest observed in the square wells, finite depth, particle-to-particle interactions, and impurity interactions break the symmetries that make different states orthogonal. Observation of this peak results in the determination of the ΔHH_{13} spacing. While the technique used to extract band offset from the spectra of parabolic quantum wells is unavailable here (there is no explicit Q_c dependence in subband spacing for square wells), fitting the transition energies and available subband spacing, using Q_c as a fitting parameter, resulted in an average value of $Q_c=0.61$ for these samples. This is in good agreement with the value determined from the parabolic samples.

The examination of square well samples is also useful as a check on the value used for the heavy hole mass in calculations. The confinement and subband spacing for heavy hole states is sensitive to the value of the effective mass. Calculations yield results consistent with observation when the Luttinger effective mass ($m_{hh}^* = 0.25m_0$) is used, supporting the use of this value in parabolic calculations.

Determination of band offset can be accomplished in ways other than those discussed above. One method is based on the position of the LH1-CB1 transition relative to the HH2-CB2 peak as well width is varied. Each peak shifts to lower energy as well width is increased, but the light hole shifts to lower energies at a lower rate than the heavy holes. This means that the peaks should cross at some well width. Using the average $Q_{cb}=0.61$ found for the square wells, Figure 7-12 plots the calculated energies of the HH1-CB1, HH2-CB2 and LH1-CB1 transitions as a function of well width.

The HH2-CB2 and LH1-CB1 transitions are predicted to cross at approximately 330Å. Open symbols correspond to experimental data, and correspond well with the predicted curve. Though unable to grow completely strained samples with well widths beyond 275 Å, spectra that include results from partially relaxed (~70% strain) samples do show that the crossing occurs between 300 Å and 350 Å well widths.

7.5 Discussion

Another method for determining band offset for a particular material system is based on an empirical rule of transitivity, which assumes that the properties of the individual semiconductors are what determine band offsets [33]. It states that the (heavy hole) valence band offset for semiconductors A, B, and C follow the rule: $\Delta E_{hh}(A/C) = \Delta E_{hh}(A/B) + \Delta E_{hh}(B/C)$. This method requires that the valence band energy of all semiconductors be measured relative to a set point - generally another semiconductor whose valence band position is set to zero. While purely empirical, this rule seems to hold for a large number of material systems.

No other work appears to have been done on the $InSb/Al_xIn_{1-x}Sb$ system, but transitivity has been used to estimate the valence band offset for $InSb/AlSb$. The purpose of using the valence band is that its offset should be independent of whether the system is direct gap or - as in the case of $InSb/AlSb$ - indirect gap. Estimates range from $\Delta E_{hh} = 0.32eV$ ($Q_v=0.22$) to $\Delta E_{hh} = 0.44eV$ ($Q_v=0.30$) (see Ichii [44], and references therein). If the offset ratio for this system, $Q_v=0.38$, is independent of

aluminum concentration over the whole range, then it would indicate a valence band offset of $\Delta E_{hh} = 0.56 eV$ for $InSb/AlSb$, which is higher than other estimates.

7.6 Conclusions

In conclusion, a conduction band offset ratio of $Q_c = 0.62 \pm 0.04$ for the $InSb/Al_xIn_{1-x}Sb$ material system has been determined. It was found to be independent of strain and aluminum concentration over the range studied ($x = .02 - 0.15$) and exhibits minimal dependence on well width. This result has been verified through examination of strained, unstrained and partially strained parabolic quantum wells, square wells, and calculations based on the crossing of heavy hole and light hole excitons with well width in square well systems. Extrapolation to the valence band offset of $InSb/AlSb$ yields a result higher than previously estimated ($\Delta E_{hh} = 0.56 eV$), yet considering the range of those estimates - and the variety in estimates for the well studied $GaAs/AlAs$ system ($Q_v \sim 0.30 - 0.40$) [45] - not inconceivable.

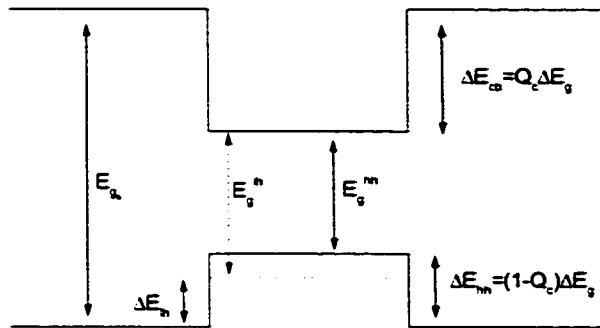


Figure 7-1 Band Offset in Square Wells

Simple diagram of the partitioning of the valence and conduction bands in a square well.

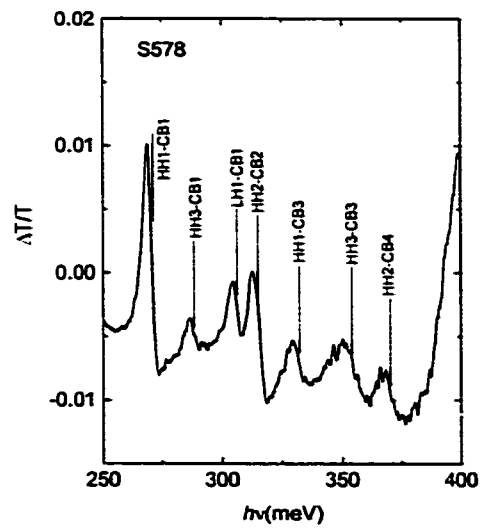


Figure 7-2 Difference Spectrum of 500Å Parabolic Quantum Well

Difference spectrum of sample S578. Note there are numerous $\Delta n=2$ transitions, which are essential to the analysis carried out.

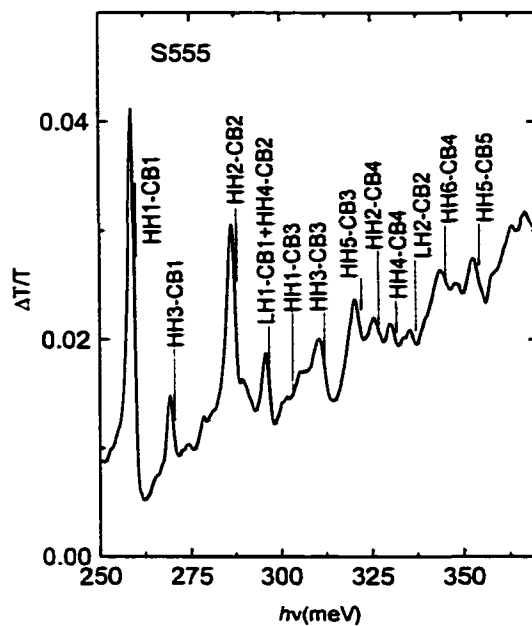


Figure 7-3 Difference Spectrum of 1000Å Parabolic Quantum Well

Difference spectrum of sample S555. This sample is twice as wide as that in Figure 7-2, with many more exciton transitions.

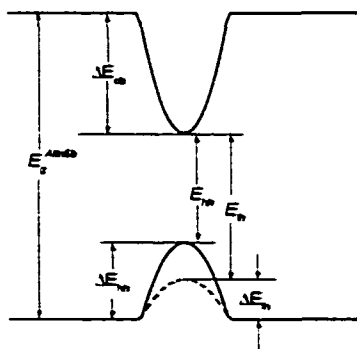


Figure 7-4 Potential Profile of a Parabolic Quantum Well

Simplified schematic of the potential energy profile of a parabolic well. Note that the digital nature of real parabolic wells is not represented here.

Table 7-1 Parameters of Parabolic Quantum Well Samples

Lister parameters are: aluminum concentration (x), well width (L_w), barrier width (L_b), whether the well or barrier is strained, and the determined offset ratio (Q_c).

Sample #	x (%)	L_w (Å)	L_b (Å)	Strain condition	Q_c
S606	2.30	1000	500	Well strained	0.63 ± 0.03
S635	3.54	1000	500	Well strained	0.60 ± 0.02
S557	5.74	1000	500	Well strained	0.60 ± 0.03
S634	6.67	1000	500	Well strained	0.65 ± 0.04
S555	8.72	1000	500	Well strained	0.63 ± 0.03
S578	8.74	500	500	Well strained	0.59 ± 0.05
S607	11.2	400	500	Well strained	0.62 ± 0.05
S638	2.01	1000	300	Barrier strained	0.59 ± 0.04
S637	5.70	1000	300	Barrier strained	0.57 ± 0.03
S580	12.06	500	500	Well 15% relaxed	0.63 ± 0.04
S575	12.12	1000	500	Well 50% relaxed	0.66 ± 0.04
S568	14.38	1000	500	Well 50% relaxed	0.64 ± 0.05
S579	14.49	500	500	Well 30% relaxed	0.63 ± 0.03

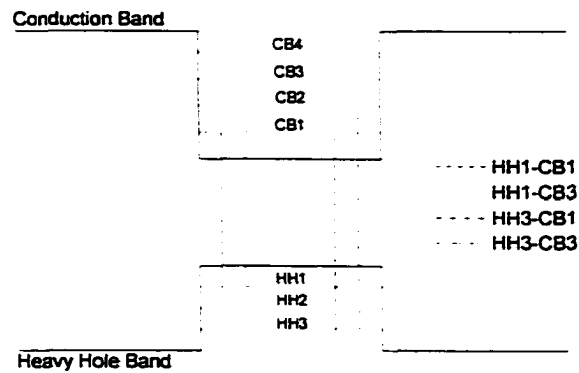


Figure 7-5 Valence to Conduction Subband Transitions

Representation of exciton transitions.

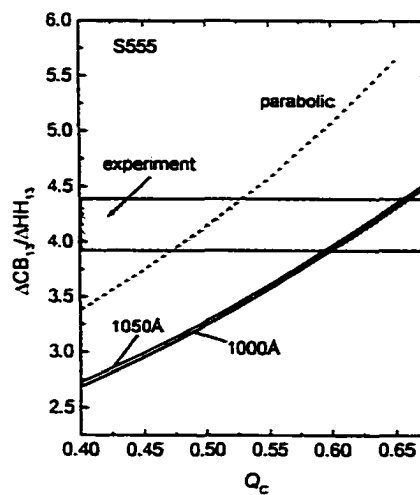


Figure 7-6 Subband Spacing Ratio Versus Offset

The solid curves are numerically calculated based on the structure of 1000Å wells that were grown. The closeness of the 1050Å curve to that for a 1000Å well demonstrates that slight variations in thickness only slightly alter results. True wells do differ significantly from ideally parabolic wells (the dashed line in the figure). The intersection of the measured ratio to that which is numerically calculated yields the results for Q_c .

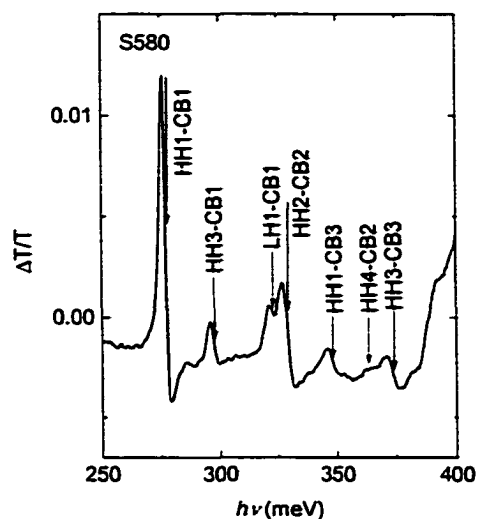


Figure 7-7 Difference Spectrum of Partially Relaxed S580

In sample S580, the well is approximately 15% relaxed. Differences in transition energies from sample S578 are accounted for by strain effects and different barrier heights.

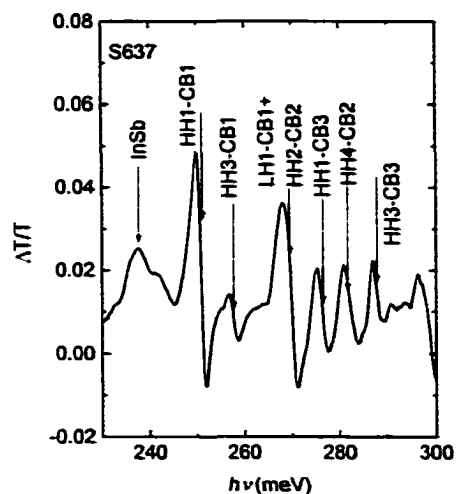


Figure 7-8 Spectrum of S637

Sample S637 is barrier strained. In this sample, a thick InSb layer is grown prior to depositing the well, which accounts for the InSb peak seen at 240 meV.

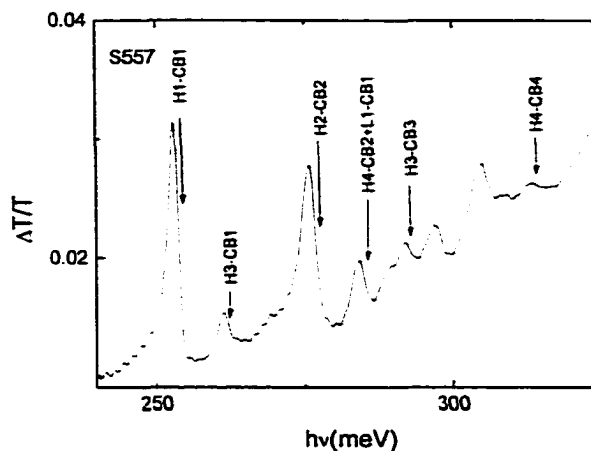


Figure 7-9 Spectrum of S557

Sample S557 is practically identical to sample S637 (Figure 7-8) except that it is well strained. The strain has shifted transitions to higher energies.

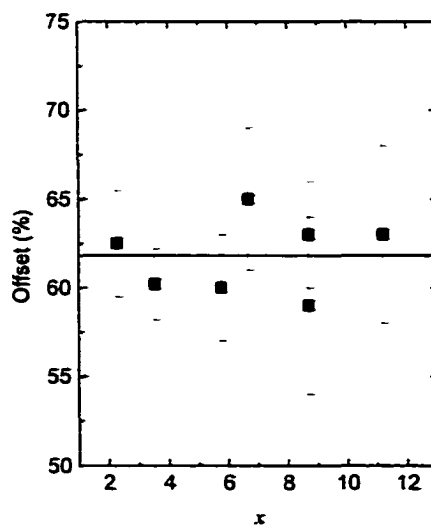


Figure 7-10 Offset versus Concentration

Plot of the determined Q_c 's for the completely strained parabolic wells as a function of aluminum concentration. The lack of variation with concentration indicates that either offset does not depend on concentration and strain in this region or that any dependence is cancelled by strain effects.

Table 7-2 Square Well Samples

Sample Number	Well Width (Å)	Aluminum Concentration (%)
S589	225	9
S595	250	9
S584	275	9

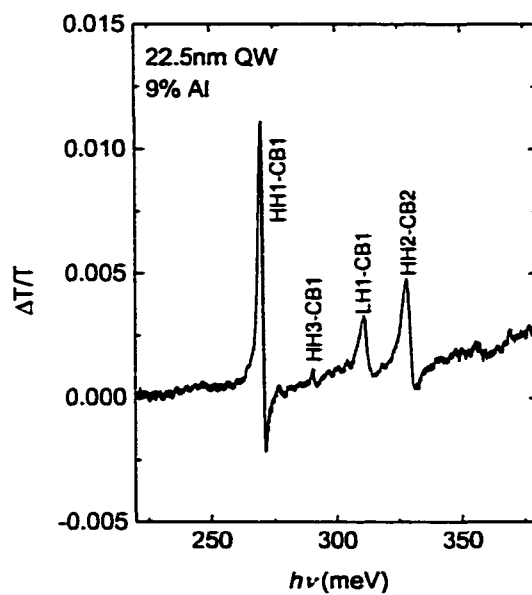


Figure 7-11 Spectrum of S589

Sample S589 is a 225Å MQW with 9% aluminum in the barriers.

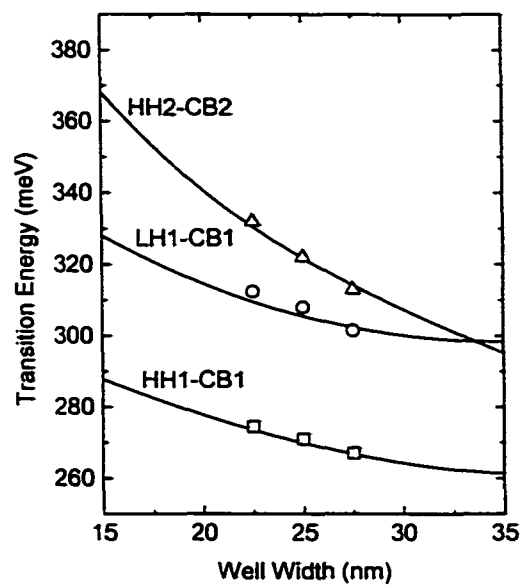


Figure 7-12 LH1-CB1 Cross Over With HH2-CB2

Calculated transitions as a function of well width. Symbols are for measured data. Samples with well widths above 275Å were partially relaxed.

Chapter 8: Determination of Deformation Potential

8.0 Introduction

The growth of heterostructures based upon semiconductors with different lattice constants introduces strain into either one - or both - of the materials. This strain can be accommodated in one of two manners: either by relaxation through the formation of defects (misfit dislocations), or by one or both of the materials elastically deforming to a new lattice constant. The amount of strain in a material that has not

relaxed is given by $\varepsilon = \frac{\delta a}{a} = \frac{a_{strained} - a_{bulk}}{a_{bulk}} = \frac{(a_{InSb}(1-x) + a_{AlSb}x) - a_{InSb}}{a_{InSb}}$, where x

is the aluminum concentration (when used in reference to $Al_xIn_{1-x}Sb$ alloys) and the “a’s” are the lattice constants of the alloy, bulk $InSb$, and bulk $AlSb$. Whether a material that is under strain relaxes or not (and to what degree) depends on its critical thickness as discussed in Chapter 4. The critical thickness for strain relaxation depends on the material. For the $InSb/Al_xIn_{1-x}Sb$ material system, Figure 4-5 plots the critical thickness of $InSb$ layers between $Al_xIn_{1-x}Sb$ as a function of aluminum concentration. The reason no (or fewer) defects form below this thickness is that it takes more energy for them to form than it takes for the $InSb$ (or whichever material one is interested in) to elastically strain to the lattice constant of the alloy.

The ability to grow layers with precision on the order of one monolayer - which is a result of advances in crystal growing technologies such as MBE - has broadened the range of material systems researchers can study. The early work in quantum wells by

Dingle and others was limited to systems in which the components were nearly lattice matched, such as $GaAs / Al_xGa_{1-x}As$, so as to avoid strain induced defects due to the relative thickness of early quantum wells. Refined growth techniques have greatly reduced the scope of this limitation, enabling the use of materials with greater lattice mismatch in the growth of strained layers. The advantages of this are many. The occurrence of misfit dislocations can severely degrade electronic properties such as mobility [15], reducing the viability of the material system for engineering applications. Accommodating lattice mismatch by elastic deformation alleviates this problem. Since the electronic and optical properties of quantum well systems are dependent on the bulk properties of the constituents, they can be designed within limits by the choices of various materials. Band gaps can then be engineered by these choices since strain induces a shift in relative band positions.

8.1 Background

8.1.1 Theory

To understand the effects of strain on the band structure of diamond/zincblende type semiconductors, one needs to differentiate between the hydrostatic and shear components of strain. In the absence of strain, the valence band edge at $\vec{k} = 0$ is four-fold degenerate. This is typical of III-IV semiconductors and is shown in Figure 2-1. Hydrostatic strain in a material changes the volume of the crystal, but not the symmetry. On the other hand, shear strain does alter crystal symmetry. For crystals layers grown along the (001) direction, the cubic structure of the strained layers is

altered by compressive or tensile strain in the layer plane. Instead of having lattice constants equal in the three directions, the two in-plane lattice constants deform so as to match those of the adjacent layers and, the lattice constant in the growth direction elongates or shortens so as to (approximately) preserve the volume of the unit cell. This strain in all three lattice directions results in both hydrostatic and shear strain dependent shifts in the relative positions of the conduction band and valence bands.

The energy shifts due to in-plane strain can be described in terms of the elastic constants - C_{ij} - and deformation potentials, which are defined as the energy shift per unit strain for electronic levels. For zincblende type crystals grown in the (001) direction, there are a number of deformation potentials, each applying to the shifts of specific bands due to either hydrostatic or shear strain. The hydrostatic deformation potentials are denoted here as “ a_c ” and “ a_v ”. They relate to the hydrostatic components of the energy shift on the conduction and valence bands, respectively. For shear strain perpendicular the (001) growth direction, one has the deformation potential “ b ”.

In terms of the above quantities, the shifts in band energies have three main components: $\delta E_{H,c}$ and $\delta E_{H,v}$ for hydrostatic effects, and $\delta E_s^{(001)}$ for shear effects on the conduction and valence bands. These terms describe the new conduction and valence band gaps by:

$$E_g^{hh} = E_0 + \delta E_{H,c} + \delta E_{H,v} + \delta E_S^{(001)}$$

Equation 8-1

$$E_g^{hh} = E_0 + \delta E_{H,c} + \delta E_{H,v} + \frac{\Delta_0}{2} \left(1 - \frac{\delta E_S^{(001)}}{\Delta_0}\right) - \frac{\Delta_0}{2} \left[1 + 2 \frac{\delta E_S^{(001)}}{\Delta_0} + 9 \left(\frac{\delta E_S^{(001)}}{\Delta_0}\right)^2\right]^{\frac{1}{2}}$$

Equation 8-2

where $\delta E_{H,c} = a_c(2 - 2\frac{C_{12}}{C_{11}})\varepsilon$, $\delta E_{H,v} = a_v(2 - 2\frac{C_{12}}{C_{11}})\varepsilon$, $\delta E_S^{(001)} = -b(1 + 2\frac{C_{12}}{C_{11}})\varepsilon$, Δ_0 is

the spin-orbit splitting at $k=0$, and E_0 is the unstrained band gap. Expanding the last

term of Equation 8-2 to first order in $\frac{\delta E_S^{(001)}}{\Delta_0}$ as $(1+x)^{\frac{1}{2}} \approx 1 + \frac{x}{2}$ yields the following

expressions:

$$E_g^{hh} = E_0 + [a(2 - 2\frac{C_{12}}{C_{11}}) - b(1 + 2\frac{C_{12}}{C_{11}})]\varepsilon$$

Equation 8-3

$$E_g^{hh} = E_0 + [a(2 - 2\frac{C_{12}}{C_{11}}) + b(1 + 2\frac{C_{12}}{C_{11}})]\varepsilon - \frac{9}{4\Delta_0} b^2 (1 + 2\frac{C_{12}}{C_{11}})^2 \varepsilon^2$$

Equation 8-4

where $a = a_c + a_v$. The hydrostatic terms have the effect of shifting the band gap of the material from its bulk value, increasing it for compressive strain and decreasing it for tensile strain. As crystal symmetry is unaffected by hydrostatic strain, it has no effect on the $\vec{k} = 0$ degeneracy of the valence bands. It is the shear term that splits the degeneracy of the heavy and light hole bands by reducing symmetry. A detailed

discussion on the derivation of these strain terms is carried out by Pollak [46]. Note that in these expressions, confinement effects (multiple energy levels and shifts in relative positions due to well width and depth) are not taken into account. Therefore, confinement energies of electrons and holes must be subtracted from observed exciton energies prior to applying these equations, which is discussed in more depth in section 8.1.3.

8.1.2 Samples

The purpose of this portion of the research is to better determine the hydrostatic and shear deformation potentials, “a” and “b” for *InSb*. Currently, accepted values are $a = -7.7$ and $b = -2.05$ [12]. This value for “b” is consistent among numerous studies, but determination of “a” has varied, with an average of $a = -7.3$ [45]. So as to be able to determine “a” and “b” for *InSb*, a series of square 50Å and 100Å multiple quantum wells were grown in which the wells were under differing amounts of strain. These samples are in addition to data from 225Å, 250Å, and 257Å multiple quantum wells. Figure 4-2 is a schematic of one such sample. The degree of strain being determined by aluminum concentration, thin wells were chosen so that a large range in x could be covered. The samples had nominal aluminum concentrations of $x=0.05$ to $x=0.30$ for the 50Å samples and $x=0.08$ to $x=0.20$ for the 100Å samples. Higher concentration samples were not grown since it was necessary that all the layers were within the region where strain is accommodated by elastic deformation of the *InSb* layers rather than misfit dislocations. Verification that the samples were fully strained was via 2D x-ray scans as discussed in Chapter 5. Figure 5-3 through

Figure 5-5 are area scans of the higher concentration samples. The elongation of the *InSb* peak in Figure 5-4 and Figure 5-5 is due to the limited thickness of the *InSb* layers in the samples. The positions of the main peaks immediately above the *InSb* tail are consistent with theoretical unstrained position of the $Al_xIn_{1-x}Sb$ alloys for the respective concentrations. Sample preparation was as detailed in Chapter 4.

8.1.3 Method of analysis

The deformation potentials for *InSb* cannot be directly extracted from excitonic spectra. The spectra show transition energies determined by subband position difference between the conduction and valence bands. Thus, the transition peak energy includes the contribution of confinement from both the valence and conduction bands. This confinement energy is dependent on both well width and barrier height and is not directly observable.

Determination of the deformation potentials starts with the measured HH1-CB1 and LH1-CB1 transition energies for each sample. These are listed in Table 8-1 for the 50Å samples and Table 8-2 for the 100Å samples. Errors due to the transition width and precisely locating the energy are also included. The process of finding the deformation potentials “a” and “b” is carried out in *Fit.cpp*, a C++ program, given in Appendix D. The first step is to read in a set of parameters for initial values. These are the observed transition energies (with errors), aluminum concentration, number of monolayers of *InSb* making up the well, the bulk band gap of *InSb*, and the initial values of “a” and “b” (the Landolt-Bornstein values are used as a first estimate).

Additional parameters determine whether to do statistical iterations based on random distributions on measured energies (which will be explained below) and whether to hold the bulk band gap as a numerical constant during fits to the data, or adjust it based on best linear and nonlinear fits. These parameters are read into the program from a file called “samples.in” which is listed in Appendix D.

It should be noted that the quantum well width is not one of the parameters listed for the program. Rather, the well width is determined from the aluminum concentration and the number of monolayers (noting that one monolayer of indium plus one monolayer of antimony has the thickness of the *InSb* lattice constant). The reason for this is to avoid the assumption that the lattice constant of the *InSb* remains constant in the growth direction regardless of the degree of in plane strain. Rather, it is assumed that the volume of the cubic cell remains approximately constant, given no misfit dislocations. This means that the actual well thickness depends on the in-plane lattice constant, which is a function of the aluminum concentration. The equation that is used in the program to determine the lattice constant in the growth direction is

$$a_z = \frac{a_{InSb}^3}{2 * a_{Al,In_{1-x},Sb}^2}$$

Equation 8-5

Multiplying this by the number of monolayers gives the well width for each sample.

As a parameter that can be varied, one can test the dependence of “a” and “b” versus well width.

For the 50Å wells, the target during growth was for 15 monolayers to be deposited per well. This corresponds to well widths between 48.8Å to 50.3Å as aluminum concentration is varied from 5%-30%. If the target growth is off by one monolayer, the widths vary between 45.6Å-53.7Å, which is approximately an 8% deviation from the goal of 50Å. For the 100Å wells, the target during growth was for 31 monolayers to be deposited per well. This corresponds to well widths between 101.3Å to 102.6Å as aluminum concentration is varied from 8%-20%. If the target growth is off by one monolayer, the widths vary between 97.9Å-105.9Å, which is approximately a 2%-6% deviation from the goal of 100Å. Variations in width due to the temperature difference at room temperature and ~4.2K observation are only about 0.2Å.

Having set initial values from “samples.in”, the program then proceeds to solve for confinement energies for the heavy and light holes for each sample. The calculation of confinement energies uses a program based upon a four-band model that accounts for band non-parabolicity and uses the previously determined band offset ratio ($Q_c=0.62$) for the conduction band [39]. The determined values for confinement energies are then subtracted from the observed transition energies, giving “theoretical” values for the heavy hole and light hole band gaps. Subtracting the strain dependent expression for the light hole gap from that of the heavy hole (Equation 8-2 from Equation 8-1) gives a nonlinear expression that is only dependent on the strain deformation potential, “b”. Note that this uses Pollaks’ full expression (Equation 8-2) for the light hole gap. Applying a nonlinear fit determines a new value for “b”.

The new value of “b” is then put into the heavy hole expression (Equation 8-1) and a series of gap values are generated that are linear versus concentration, and depend only on “a”. Using a linear fit to these values generates a new value for “a”. If the parameter to re-evaluate the bulk band gap for *InSb* is turned on, then the intercept of this line gives a new $E_{g_{InSb}}$. Otherwise, the bulk *InSb* gap remains constant. The loop is then started over with the new “a”, “b”, and possibly $E_{g_{InSb}}$, if so chosen. The iterations continue until the convergence criteria for “a” and “b” are met, in this case

$$\left| \frac{old - new}{old} \right| < 0.0001 \text{ for each parameter.}$$

The above iterative routine is the heart of the analysis for finding “a” and “b”. The next step is to assign error bars to the values found. Initial errors are based on the uncertainty in the assignment of transition energies for heavy and light holes. Based on the assumption that two identical measurements would yield slightly different energies, the program generates a random Gaussian distribution of possible measured energy values within the measurement error. The number of loops is a parameter in “samples.in”, so can be varied by choice. This creates a list of different (converged) values for “a” and “b”. The standard deviation and mean of “a” and “b” are then taken. The results given below are the mean values, with errors being the standard deviation.

8.2 Results

Through a detailed analysis of results, it has been determined that the 50 Å samples are too thin to yield reliable results for the deformation potentials. A number of factors come into play in interpreting the results for the analysis of the 50 Å samples. The measured transition energies that are fed into the analysis are reliable, though the error associated with each due to the width of the transition peak lend to some uncertainty in the results. Two factors that have the most significant affect on the predicted values of “a” and “b” are the number of monolayers that compose the quantum wells, and the true value of the bulk band gap of *InSb*. Values of “a” ranged from about $a = -7.84$ to $a = -10.03$ for the 50 Å samples and from $a = -7.72$ to $a = -7.84$ for the 100 Å samples. The errors for “a” were consistently around 0.45 with gap feedback and 0.37 without gap feedback for the 50 Å samples and 0.17 with gap feedback and 0.11 without gap feedback for the 100 Å samples. The results for “b” ranged from -1.99 to -2.09 , with errors of about 0.15 both with and without gap feedback for the 50 Å samples and from -1.92 to -1.93 with errors of about 0.045 for the 100 Å samples. Trends in results based on initial assumptions will be presented after a discussion of one case – that of 15 monolayers. The same trends were seen in the 31 monolayer (100 Å) samples, which will be discussed in the following section.

8.2.1 15 Monolayers

For each of the results listed in Table 8-3 – Table 8-5, a total of 1024 runs were carried out to provide a large sample size for determining mean values and standard deviations. Figure 8-1 through Figure 8-4 graphically depict this data. When error

bars are excluded from the plot of “a”, a linear trend is noted when gap feedback is turned off. This is seen to a lesser degree when the same is done with the “b” plot. The best agreement between runs holding the gap fixed and feeding it back into the new calculations comes at a bulk band gap of 0.240eV from the plots of “a” and 0.239eV from the plot of “b”. As the error in “b” is much less than that of “a”, a bulk band gap value of 0.239eV appears most reasonable when a well thickness of 15 monolayers is assumed.

8.2.2 Trends

When the *InSb* band gap is held constant, the tendency for the predicted “a” value to vary linearly with band gap occurs for each set of runs based on the number of monolayers assumed. Likewise, “b” shows a (weaker) linear trend. For each set of runs, when gap feedback is turned on, “a” and “b” are relatively constant regardless of the number of monolayers and of the initial estimate of zero concentration band gap. Additionally, the calculated band gap of bulk *InSb* depends strongly on the number of monolayers, and is consistent regardless of the initial assumption of its value. This is depicted in Figure 8-5. For the sake of clarity, error bars have been excluded from this figure. The error in these calculations runs from 0.002302eV to 0.002486eV.

8.2.3 31 Monolayers

Table 8-6 through Table 8-8 list the results for the 31 monolayer samples. Figure 8-6 through Figure 8-9 graphically depict this data. As with the 15 monolayer samples,

when error bars are excluded from the plot of “a”, a linear trend is noted when gap feedback is turned off. This is seen to a lesser degree when the same is done with the “b” plot. The best agreement between runs holding gap fixed and feeding it back into the new calculations comes at a bulk band gap of 0.237eV from the plots of “a” and 0.236eV from the plot of “b”. The error in “b” is less than that of “a”, but by a smaller margin than with the 15 monolayer samples. A bulk band gap value of between 0.236eV and 0.237eV appears reasonable when a well thickness of 31 monolayers is assumed. Figure 8-10 depicts the calculated band gap dependence on the number of monolayers assumed. The error in these calculations runs from 0.000689eV to 0.000719eV.

8.3 Discussion

For the 50Å wells, error bars are large enough to yield any conclusions as to the values of the deformation potentials meaningless. While the predicted values of the shear deformation potential “b” are relatively unaffected by the initial assumptions of band gap and number of monolayers, there is a large discrepancy between those calculated for “a” (around -8.97) and the accepted value of -7.7. Of note is that the results for each reduces in magnitude as the number of monolayers is reduced. This same behavior is seen for the predicted band gap.

As a test of these calculated results, heavy and light hole band gaps were numerically calculated for 3 wide well samples, with quantum wells widths of 225Å, 250Å, and 275Å. Numerical predictions of observed exciton peaks for these wells are in good

agreement with observation when the values of $a=-7.7$ and $b=-2.05$ are used. Using the values based on 50Å wells, however, yield numbers inconsistent with observation. Additionally, comparing just the heavy and light hole band gap versus barrier aluminum concentration (i.e. versus strain), the wide well gaps do not fit on the curve generated by the thin wells. Figure 8-11 is based on the values of “a” and “b” calculated with an assumption of 15 monolayers. The predicted heavy and light hole lines are plotted. As might be expected, the thin well heavy and light hole points are in good agreement with the curve. That wide well points do not agree with the predicted curve (remembering that all the points plotted are initially based on observed energies) indicates that these values for “a” and “b” cannot be correct.

Repeating this procedure for each of the predictions based on different numbers of monolayers (± 1 monolayer from the growth target of 15) does not lead to agreement between thin and wide wells, though an analysis assuming 14 monolayers yields closer results, as can be seen in Figure 8-12. While the converged band gap estimate from this analysis is reasonable at 0.237eV, the high value of $a=-8.14$ and lack of consistent results when considering the wide wells again indicates that these results cannot be correct. The results from the 16 monolayer analysis were worse than those for 15 monolayers. They are presented in Figure 8-13. As with the above two analyses, these results cannot be correct due to the discrepancy with wide well data. Additionally, the predicted band gap assuming 16 monolayers is 0.242eV, which is above even the highest of current estimates.

Repeating this analysis for the results obtained from the 100Å samples yielded results more consistent with the wide well data. When the growth target of 31 monolayers is assumed, the calculated value of $a=-7.72$ is consistent with the accepted value of -7.7 . The calculated value of $b=-1.92$ is slightly lower than the accepted value of -2.05 , but remained relatively consistent between calculations regardless of the number of monolayers assumed, whether the bulk band gap was fixed in the calculations, and the value of the band gap. Numerical predictions on the observed exciton peaks for wide well samples are in much better agreement with observations based on these calculated values than with those obtained from the 50Å samples, though they are still slightly different. Figure 8-14 is based on the values of “a” and “b” calculated with an assumption of 31 monolayers. Comparison with Figure 8-11 (which is plotted on the same scale) clearly shows much better agreement with the wide well data. Table 8-9 gives the values for the heavy and light hole band gaps for the wide wells based on Equation 8-1 and Equation 8-2 for both the 15 and 31 monolayer calculations. The numerically calculated heavy and light hole energy gaps are also presented. One can again see that the 31 monolayer results for “a” and “b” yield are more accurate when wide well data is used for comparison.

An additional analysis was carried out in which the bulk gap was kept fixed during calculations using the values of $a=-7.722$ and $b=-1.92$. The purpose was to see if a particular value of the InSb bulk band gap gave better correspondence between the wide well data and the curves generated from Equation 8-1 and Equation 8-2. These calculations were only used to determine the confinement energies of the electrons

and holes, not to try and find a new “a” and “b”. The bulk gap value that gave the closest results between the 100Å wells and the wide wells was 0.234eV, which is below slightly below current estimates for the *InSb* band gap. As a check for consistency between this value for the bulk band gap and the “a” and “b” used in its determination, a complete analysis was carried out to check if it would yield the same values for “a” and “b”. The results were inconsistent, yielding $a=-8.05$ and $b=-1.94$.

As was done in the analysis of the 50Å samples, calculations were carried out for ± 1 monolayer from 31 monolayers. Figure 8-15 shows the results assuming 32 monolayers were deposited per well during growth. The discrepancy between the wide well data and the predicted curve is larger than when 31 monolayers are assumed. The predicted bulk gap in this instance is .238eV. When 30 monolayers are assumed, the analysis yields $a=-7.46$, $b=-1.91$, and a bulk gap of 0.236eV. The discrepancy between the predicted curve and the wide well data points is about half of what it was in the 31 monolayer analysis (Table 8-10). The value for “b” is consistent with other monolayer and bulk gap assumptions and the predicted bulk gap is reasonable. The primary difference is the low result for “a”. Although lower than that listed in [12], it is in line with the value of $a=-7.3$ from [45], which is an average value from different publications.

As this methodology works well for predicting energies with wide well observations when more accepted values for deformation potential are used, the question arises as to why such different values are calculated for thin (50Å) wells. It has been

postulated by Litvinov, et. al. [47] that the deformation potentials may differ from bulk values for narrow band gap quantum wells. A condition imposed is that the well be deep:

$$\frac{m^* \Delta E_{cb} L^2}{\hbar^2} \gg 1$$

Equation 8-6

For these narrow well systems, this condition is not met as the well depth is proportional to aluminum concentration, but the width is limited by it. As an example, for a 50 Å well with $x=0.06$, one gets 0.35 for Equation 8-6 (using the same values as with the simple transmission calculation in the previous chapter). For wider wells, the condition is closer to being met (for $L=300\text{Å}$, the result is 12.55), but is still much smaller than the example used by Litvinov, et. al.

A more likely explanation has to do with the potential profile of the of the well/barrier interface. In the model used by the program, the wells are modeled as square wells. Inherent in this assumption is an abrupt interface that does not take into account the finite distance it takes to transition from $InSb$ in the well to $Al_xIn_{1-x}Sb$ in the barrier. For thin (50Å) wells, this transition distance can be an appreciable percentage of the well width. Assuming half a monolayer transition distance on each interface means a variation of well width between 6% and 7% between the bottom and top of the well. This can significantly affect the resulting energy levels detected

by the electron and hole states. With the 100Å wells this variation is only on the order of 3%, so it would have less effect.

Theoretical work on compositional grading has been done on $GaAs / Al_xGa_{1-x}As$ by Shulman [48]. The model used assumed a linear variation in the potential from well to barrier material. This model found that grading can have a significant effect on energy levels in quantum wells, and that this effect was more pronounced in thinner wells. This could seriously skew the results of calculations based on abrupt interfaces, as in the calculations performed on the 50Å wells. A variation of the barrier potential profile on the order of a monolayer would have an insignificant effect on wide (say, 200Å) quantum wells for two reasons. First, even a variation over a few monolayers is a very small amount compared to the width of the well. Second, lower confinement in wide wells may mean that the lower lying states (which are all that is used in this analysis) would experience a confining potential more in line with that produced by a square well, depending on where the potential variation starts (partially in the well or where the barrier “starts”). Another source of error is that the small binding energy of $InSb$ excitons is not taken into account in these calculations. An additional factor not taken into account are any irregularities in the well barrier interfaces, though one would expect this to – on average - broaden the observed transition rather than shift the energy.

8.4 Conclusions

The use of thin quantum wells for the determination of deformation potentials is problematic, and yields inconclusive results from 50Å samples. The results from 100Å samples more consistent with data from wider wells, but there still remains a small discrepancy. While differences between bulk and confined deformation potentials may be a factor, a more straight forward explanation is the variation in the potential profile between well and barrier (and how one defines an interface in this instance). Further analysis based on wider wells (175Å or greater) may be more conclusive, though the results from the 100Å wells are in general agreement with the currently accepted values for the deformation potentials of *InSb*. Numerical calculations taking into account the non-abrupt potential profile at the well/barrier interface may also yield more insight into the physics involved in finding the deformation potentials.

Table 8-1 Transition Energy Versus Aluminum Concentration for 50Å Samples

Aluminum Concentration (%)	HH1-CB1 transition energy (eV)	LH1-CB1 transition energy (eV)	HH1-CB1 Error (eV)	LH1-CB1 Error (eV)
4.82	0.3195	N/A	0.003	N/A
11.1	0.3779	0.4303	0.002	0.0025
20.7	0.4336	0.5393	0.002	0.007
32.2	0.4782	0.635	0.003	0.0045

Table 8-2 Transition Energy Versus Aluminum Concentration for 100Å Samples

Aluminum Concentration (%)	HH1-CB1 transition energy (eV)	LH1-CB1 transition energy (eV)	HH1-CB1 Error (eV)	LH1-CB1 Error (eV)
8	0.30536	0.34939	0.000305	0.001075
12	0.319	0.38189	0.001075	0.000345
16	0.33243	0.4146	0.000345	0.00188
20	0.34219	0.44333	0.00188	0.001085

Table 8-3 Calculated α With Error for Different Initial Band Gaps for 15 Monolayers

Initial Band Gap	a (No Gap Feedback)	sig_a (No Gap Feedback)	a (With Gap Feedback)	sig_a (With Gap Feedback)
0.236	-9.152918	0.363544	-8.976764	0.442216
0.237	-9.098778	0.369569	-8.975743	0.422658
0.238	-9.052154	0.35987	-8.952432	0.418664
0.239	-8.996162	0.356661	-8.966748	0.438718
0.24	-8.955157	0.35933	-8.962203	0.435311
0.241	-8.899479	0.355438	-8.961028	0.429574
0.242	-8.858595	0.354367	-8.984012	0.422407

Table 8-4 Calculated b With Error for Different Initial Band Gaps for 15 Monolayers

Initial Band Gap	b (No Gap Feedback)	sig_b (No Gap Feedback)	b (With Gap Feedback)	sig_b (With Gap Feedback)
0.236	-2.053706	0.14691	-2.037	0.141
0.237	-2.050871	0.150547	-2.048	0.147911
0.238	-2.041971	0.144636	-2.046	0.144027
0.239	-2.042756	0.146737	-2.043	0.148216
0.24	-2.040751	0.148581	-2.046	0.149106
0.241	-2.042394	0.144358	-2.04	0.145348
0.242	-2.038467	0.144639	-2.048	0.144358

Table 8-5 Converged Band Gap Estimates for 15 Monolayers

Eg(Initial)	Eg (Final)	Standard Deviation
0.236	0.239409	0.002467
0.237	0.239615	0.002451
0.238	0.239735	0.002408
0.239	0.23967	0.002449
0.24	0.239662	0.002379
0.241	0.239614	0.002391
0.242	0.239628	0.002375

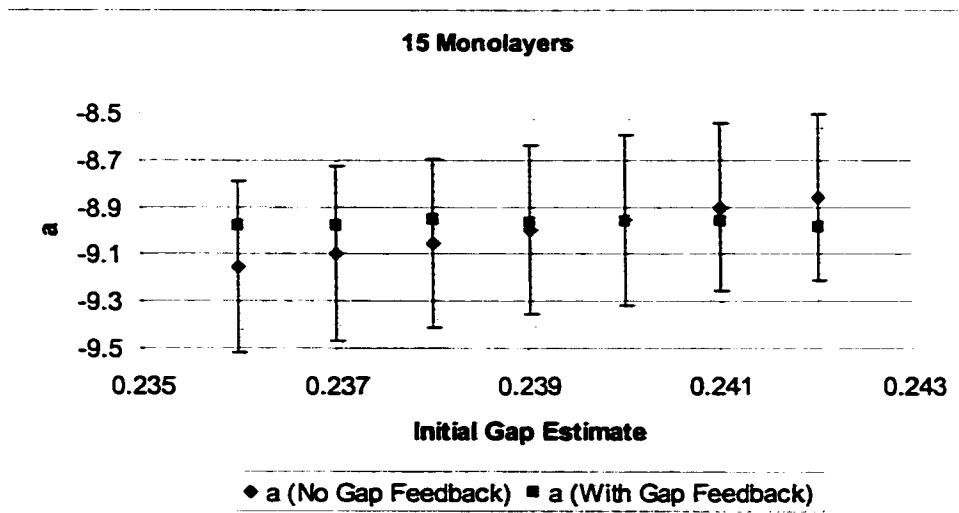


Figure 8-1 a Versus Initial Gap Estimate With Error Bars

The dependence of a on initial InSb band gap estimate is clearly seen when the gap is kept fixed rather than updated every iteration of the calculations.

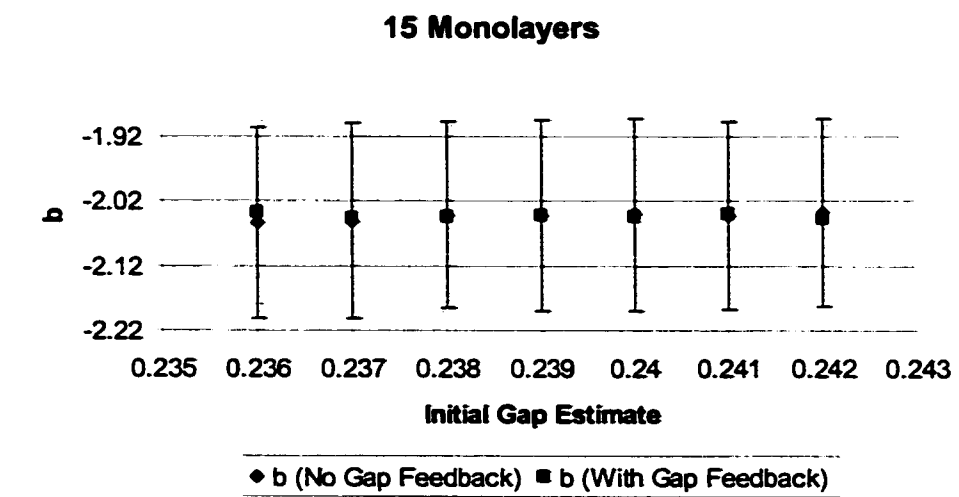


Figure 8-2 b Versus Initial Gap Estimate With Error Bars

The resulting value of b is less influenced by the initial gap estimate than that of a .

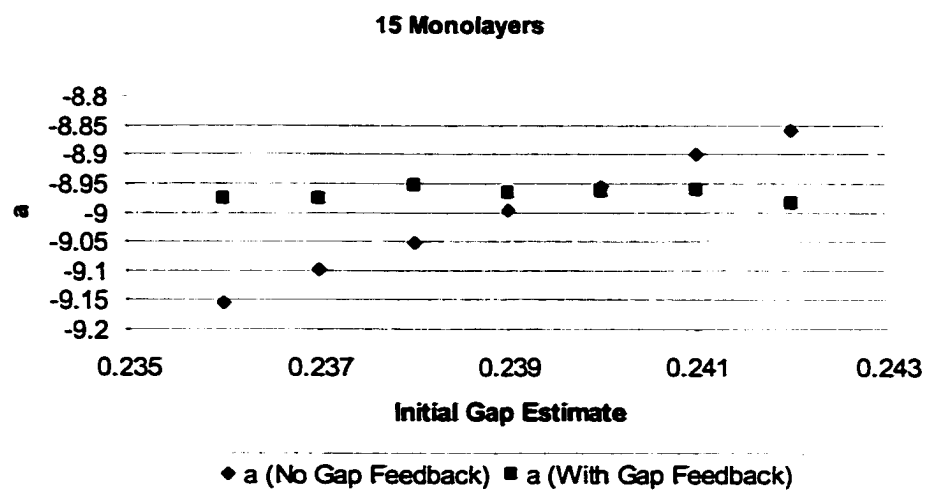


Figure 8-3 *a* Versus Initial Gap Estimate Without Error Bars

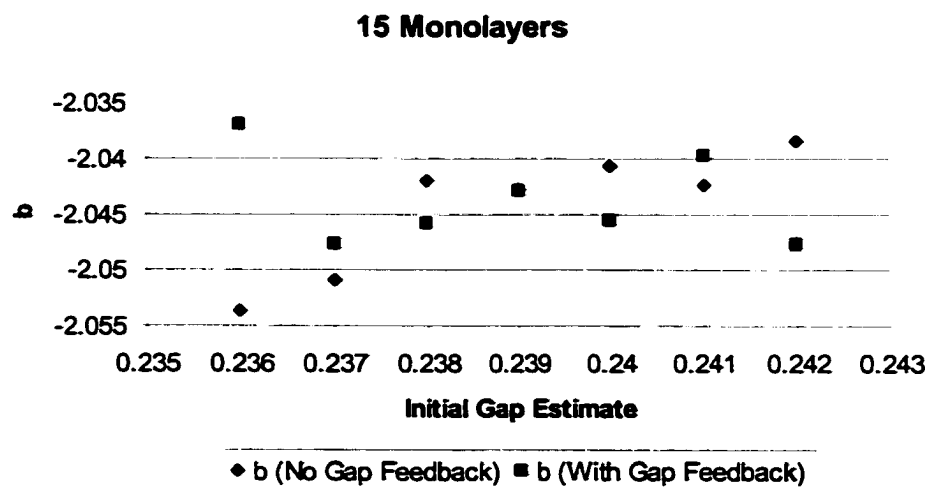


Figure 8-4 *b* Versus Initial Gap Estimate Without Error Bars

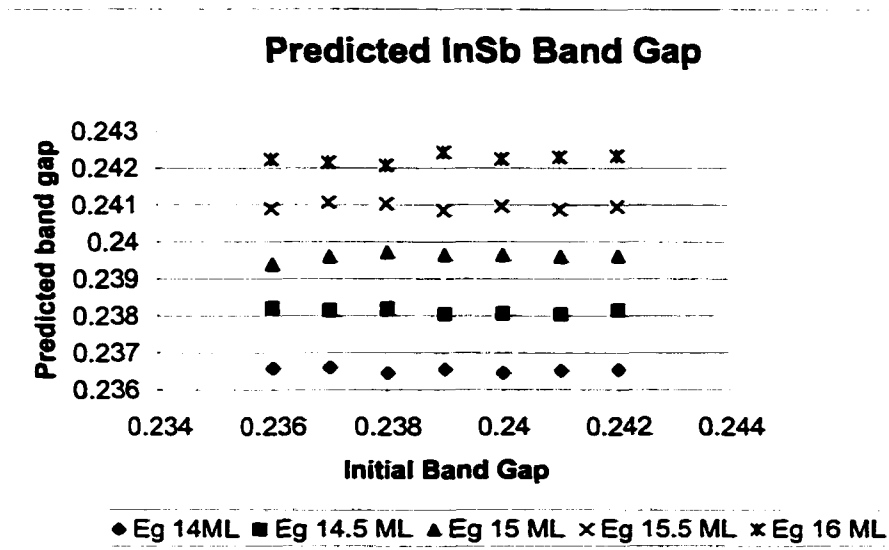


Figure 8-5 Converged Band Gap Versus Number of Monolayers

The predicted band gap shows strong dependence on the number of monolayers used in calculations.

Table 8-6 Calculated a With Error for Different Initial Band Gaps for 31 Monolayers

Initial Band Gap	a (No Gap Feedback)	sig_a (No Gap Feedback)	a (With Gap Feedback)	sig_a (With Gap Feedback)
0.236	-7.836208	0.107767	-7.726376	0.174448
0.237	-7.731954	0.116095	-7.72107	0.161574
0.238	-7.587925	0.114627	-7.698	0.173958

Table 8-7 Calculated b With Error for Different Initial Band Gaps for 31 Monolayers

Initial Band Gap	b (No Gap Feedback)	sig_b (No Gap Feedback)	b (With Gap Feedback)	sig_b (With Gap Feedback)
0.236	-1.93116	0.044661	-1.92929	0.044489
0.237	-1.93011	0.047195	-1.92376	0.045797
0.238	-1.91924	0.048144	-1.924	0.045422

Table 8-8 Converged Band Gap Estimates for 31 Monolayers

Eg(Initial)	Eg (Final)	Standard Deviation
0.236	0.236946	0.000809
0.237	0.236928	0.000692
0.238	0.237021	0.000739

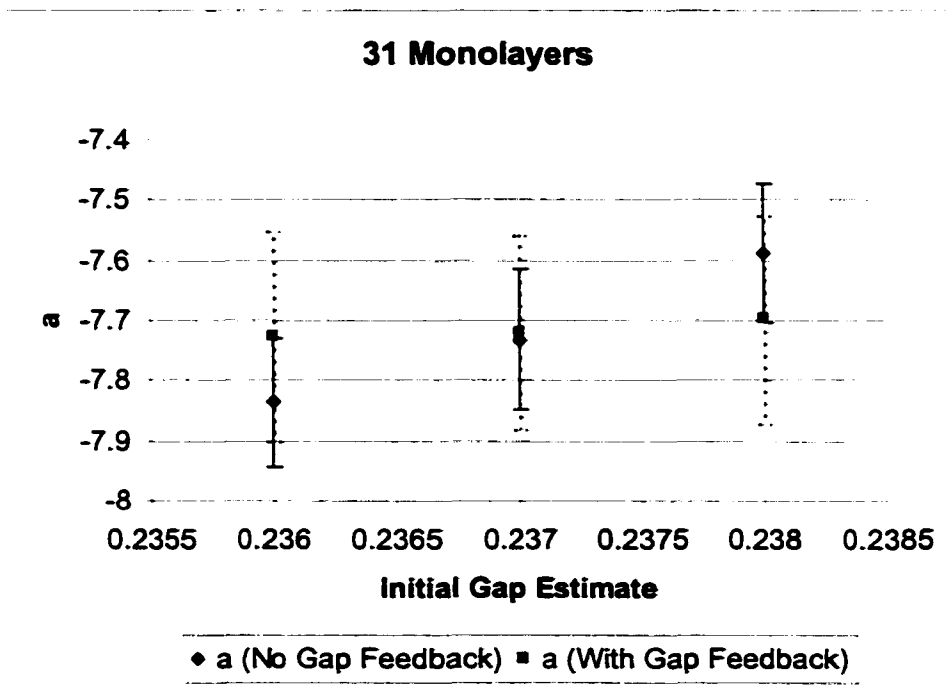


Figure 8-6 α Versus Initial Gap Estimate With Error Bars

As with the 50Å samples, α is dependent on the initial gap estimate when not iteratively updated.

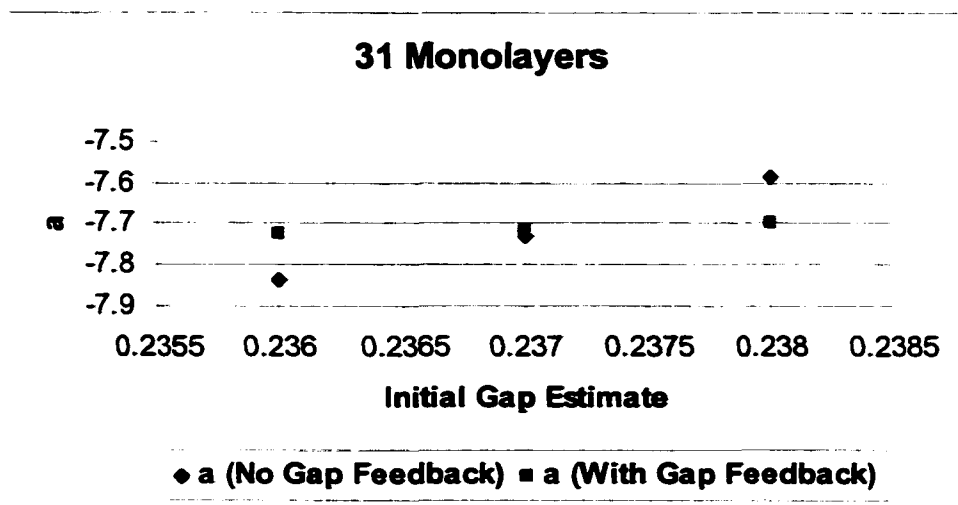


Figure 8-7 a Versus Initial Gap Estimate Without Error Bars

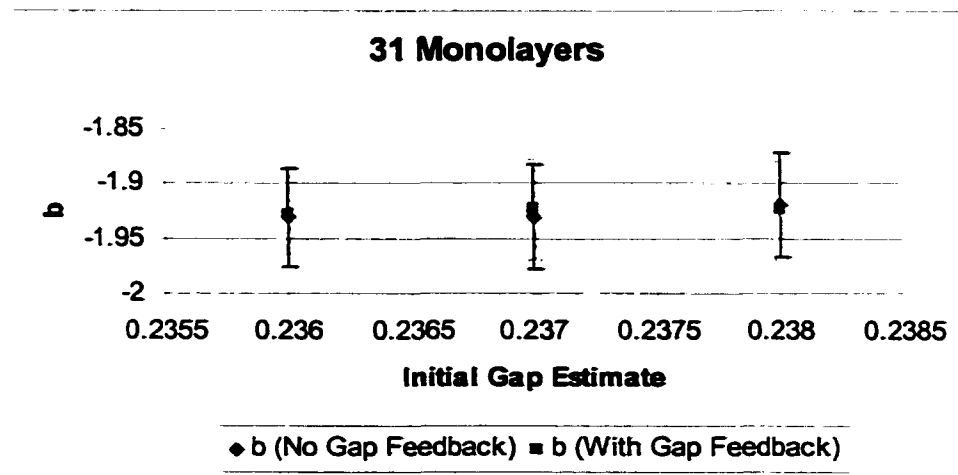


Figure 8-8 b Versus Initial Gap Estimate With Error Bars

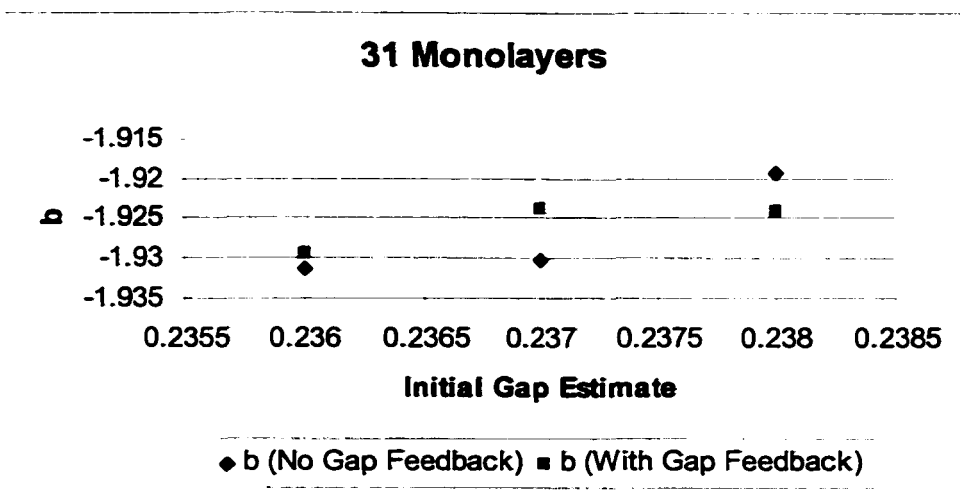


Figure 8-9 *b* Versus Initial Gap Estimate Without Error Bars

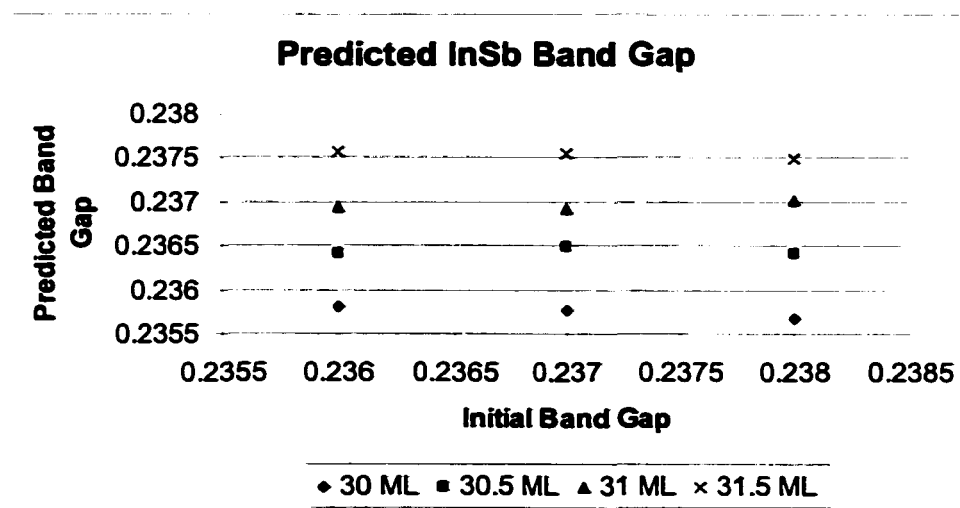


Figure 8-10 Converged Band Gap Versus Number of Monolayers

The predicted band gap depends on the number of monolayers used in the calculations.

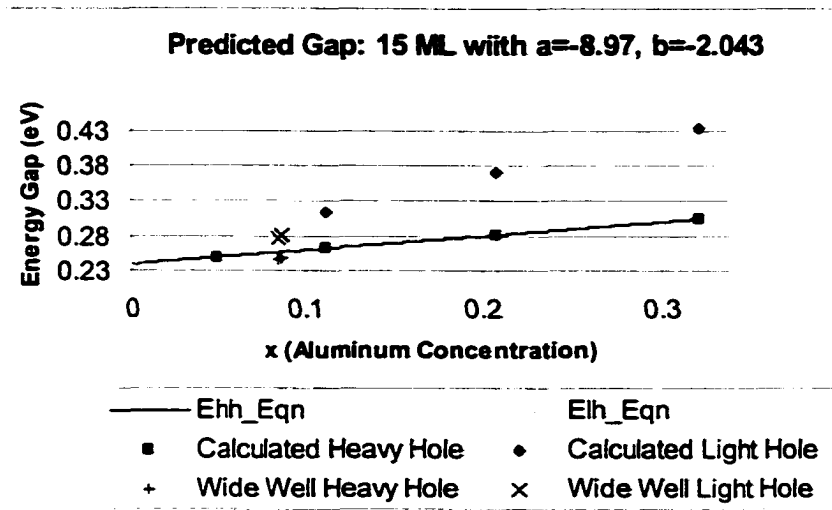


Figure 8-11 Band Gap Versus Aluminum Concentration: 15 Monolayers

Wide well energies based on this calculated a and b do not fit the predicted curve.

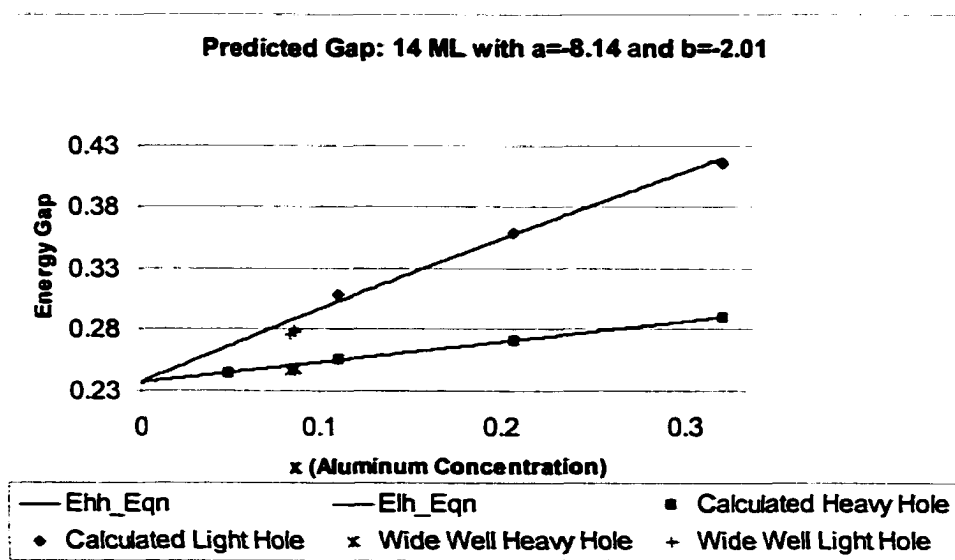


Figure 8-12 Band Gap Versus Aluminum Concentration: 14 Monolayers

Wide well energies based on this calculated a and b do not fit the predicted curve.

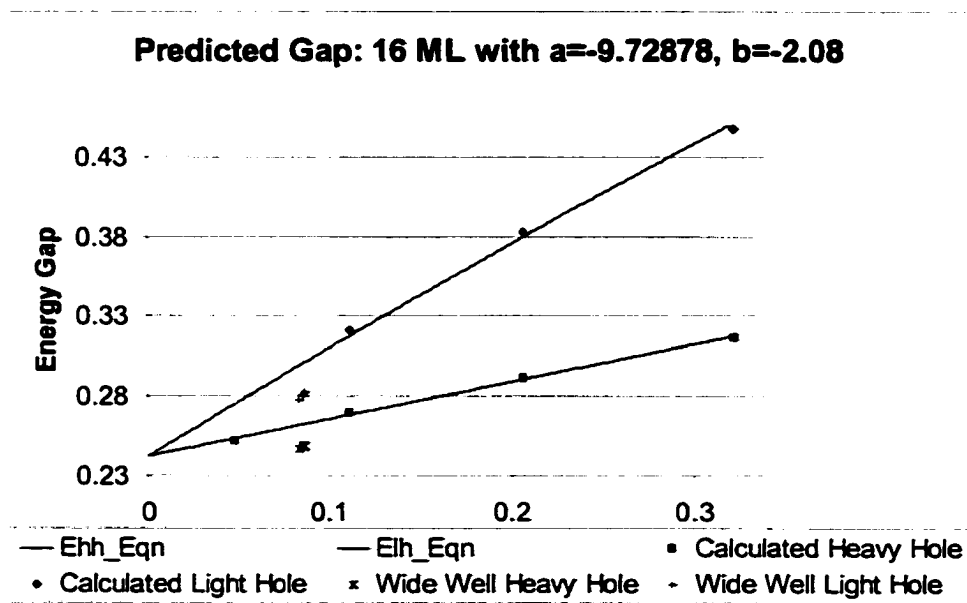


Figure 8-13 Band Gap Versus Aluminum Concentration: 16 Monolayers

Wide well energies based on this calculated a and b do not fit the predicted curve.

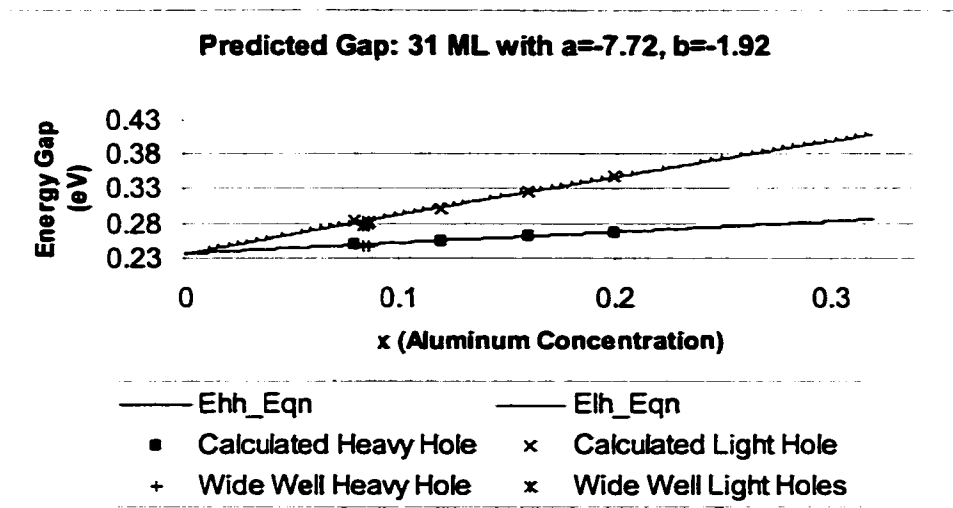


Figure 8-14 Band Gap Versus Aluminum Concentration: 31 Monolayers

Wide well results are much closer with the results based on the 100Å wells.

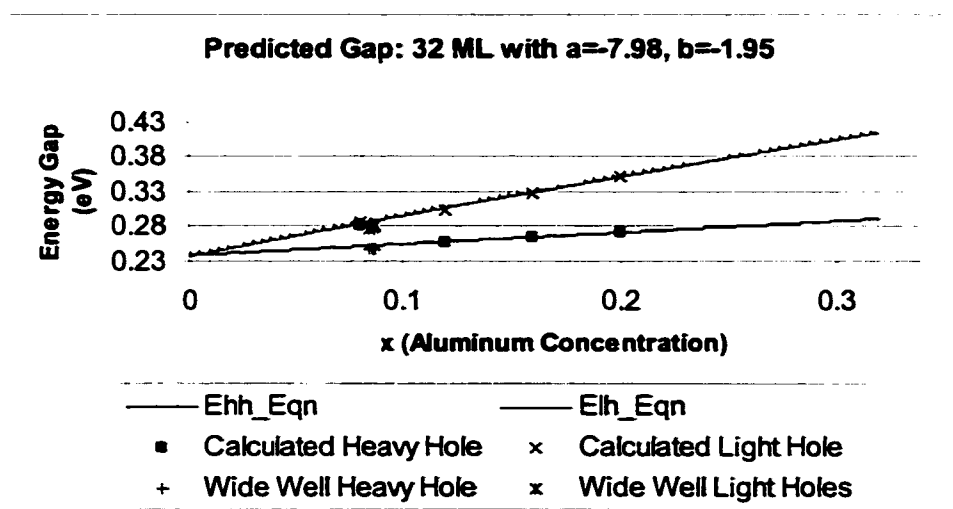


Figure 8-15 Band Gap Versus Aluminum Concentration: 32 Monolayers

Table 8-9 Difference Between Wide Well Data and Predicted Curves: 31 and 15 Monolayers

x	31 ML: Ehh_Eqn	31 ML: EgHH	HH Shift (eV) From Calculation
0.084	0.249994445	0.2469	0.003094445
0.086	0.250305551	0.24783	0.002475551
0.0866	0.250398882	0.24775	0.002648882
		Average Shift -->	0.002739626
x	31 ML: Elh_Eqn	31 ML: EgLH	LH Shift (eV) From Calculation
0.084	0.284936737	0.27647	0.008466737
0.086	0.286059747	0.27944	0.006619747
0.0866	0.286396465	0.28066	0.005736465
		Average Shift -->	0.006940983
x	15 ML: Ehh_Eqn	15 ML: EgHH	HH Shift (eV) From Calculation
0.084	0.256620324	0.24657	0.010050324
0.086	0.257023903	0.24803	0.008993903
0.0866	0.257144977	0.24798	0.009164977
		Average Shift -->	0.009403068
x	15 ML: Elh_Eqn	15 ML: EgLH	LH Shift (eV) From Calculation
0.084	0.293674279	0.27708	0.016594279
0.086	0.294937422	0.28014	0.014797422
0.0866	0.295316155	0.28147	0.013846155
		Average Shift -->	0.015079285

Table 8-10 Difference Between Wide Well Data and Predicted Curves: 30 Monolayers

x	HH Shift (eV)	LH Shift (eV)
0.0866	6.61E-04	3.56E-03
0.086	4.84E-04	4.42E-03
0.084	1.62E-03	6.27E-03
Average	9.23E-04	4.75E-03

Chapter 9: Modulation Doping and the Fermi Edge Singularity

9.0 Introduction

To this point, only undoped quantum wells have been investigated. The intentional introduction of carriers – n type (electrons) or p type (holes) - significantly affects the exciton spectra in quantum wells. This chapter will examine the observation of the Fermi Edge Singularity (FES) - known as the “Mahan Exciton” - in the $InSb/Al_xIn_{1-x}Sb$ MWQ system.

9.1 Theory

9.1.1 Doping

This portion of the research examines the effects of doping as the Fermi level is raised to the level where electrons occupy the first conduction subband. When this occurs, the features of the exciton absorption spectrum for this lowest state are drastically altered. The many-body origin of the FES – as well as its dependence on temperature and doping level - will be discussed.

The addition of n type dopants to semiconductors raises their Fermi level by increasing the number of unbound electrons. This affects the exciton spectra by altering the energy an electron must absorb to be excited to a state in the conduction band. The experiments discussed in this chapter of the dissertation were conducted on n -type samples doped with silicon. When silicon occupies an indium site, three of

the four outer shell electrons form covalent bonds with the with adjacent antimony atoms, leaving one unbound electron. The addition of electrons to the conduction band raises the Fermi level in these samples. Adjusting the doping level during MBE growth enables one to adjust the number of carriers in the sample. The method of doping is also important. With uniform doping, impurities are added both to the barrier and to the well. These impurities form scattering centers in the well that reduce mobility. The advantage in delta doping is that electrons are added only to the barrier. Delta-doping in the $Al_xIn_{1-x}Sb$ barriers allows these electrons to “drop” into the lower potential wells, thereby adding electrons to the wells while keeping scattering centers in the barriers.

9.1.2 Fermi Edge Singularity

The existence of the FES was first postulated by Mahan [49]. Although it has been referred to as the “Mahan exciton”, it is not a bound state between an electron and hole (which will be discussed below). It originates from the photo-excitation of a valence electron to the conduction band - as do excitons – but the transition does not occur at $\vec{k} = 0$. Limiting this discussion to quantum wells, the population of the first conduction subband by electrons fills available states in that subband and raises the Fermi energy. The exclusion principle prevents $\vec{k} = 0$ transitions as these electron states are already filled. The first available electron states are just above the Fermi level, which is where the FES is observed. This transition is depicted in Figure 9-1

for the $E - v_s - \bar{k}$ dispersion relation of quantum well subbands. The shaded region in the figure represents the sea of electrons, the top of which is the Fermi level.

9.1.3 Potential Profile

Many factors must be considered in examining doped quantum wells. Already mentioned is the relationship between doping level and the Fermi energy. In multiple quantum wells, the bulk electron concentration (in cm^{-3}) is equally divided among the wells so as to maintain the same Fermi level throughout the crystal. When the wells are quasi-two dimensional in nature, the concentration n is given in units of cm^{-2} . Additionally, the potential discontinuity at the well interface differs in the presence of an electron sea. What would ideally be a square profile is affected by the electrostatic interaction between the electrons in the wells and the ionized donors in the barrier. Sanders and Chang [50] have modeled the effects of modulation doping by adding a potential term to be evaluated due to modulation doping. This potential, which is considered flat in undoped wells, can be calculated self-consistently and is modeled as parabolic due to charge separation. The convention is to treat the electrostatic potential due to the ionized donor atoms in the barrier as positive and that of the negatively charged electrons in the well as negative. This is shown in Figure 9-2 [51] with the height of the bending of the potential in the well denoted as E_B . Additional features shown are the Fermi level (F_e), the level of the first conduction subband (E_c) in an undoped well, and the lowering in energy of that subband (band gap renormalization) due to the sea of electrons. Self-consistent calculations were carried

out in support of this portion of the research by Khodaparast [39] to determine the subband spacing of these doped samples. The model used is not expected to predict band gap renormalization due to the electron sea. Results of these calculations are listed in Table 9-1. Of note is that these results differ only slightly from the separations in undoped wells.

9.1.4 Many body origin

As stated, the FES is not an exciton. While there exists at least one state for any undoped quantum well regardless of its depth, the situation in the presence of a sea of electrons is very different. Kleinman [52] has shown that occupation of a subband by charged carriers precludes the possibility of any excitonic bound state involving that subband. He also demonstrated theoretically that excitons related to higher subbands not occupied by unbound carriers are still possible if the quantum well supports those higher states. This result holds true regardless of carrier density as long as the higher subband remains unoccupied. The absorption observed at the Fermi level is a collective response of the Fermi sea to both the addition of an electron and to the photo-generated, positively charged, hole.

Optical absorption in doped quantum wells is more difficult to describe quantitatively than in undoped wells, yet the prohibition against an excitonic bound state is reasonable. While each of the electrons in the occupied subband are in different quantum states due to their fermionic nature, they are identical particles. Coulombic

interactions with a hole involve all the electrons, making the formation of a bound state involving just one of the electrons energetically unfavorable.

9.1.5 Temperature

The FES, being a many body effect involving excitation to the Fermi level, exhibits a strong dependence on temperature. The occupation of states by electrons near the Fermi level is controlled by the Fermi distribution. What begins as a sharp level near 0K smears as temperature is increased due to thermal scattering of electrons at the Fermi surface. This smearing is reflected in the photo-excitation of electrons to the occupied subband. At low temperatures ($\sim 10\text{K}$), the FES absorption is a pronounced peak displaced in energy from the expected position of the HH1-CB1 exciton by approximately the difference in energy between the Fermi level and the bottom of the first subband. This is depicted in Figure 9-3, where S474 is compared to an undoped 250 Å sample (S595). These difference spectra are for 4K-30K. The left arrow on the upper curve in Figure 9-3 marks the location of the HH1-CB1 transition in an undoped well (and the HH1-CB1 separation in the doped well). The right arrow marks the predicted position of the FES (which will be discussed below). As temperature is increased, the FES transition rapidly broadens due to the smearing of the Fermi surface and decreases in intensity until it is indistinguishable (see Figure 9-7). Excitonic features such as the HH2-CB2 transition exhibit a temperature dependence that is similar to that seen in undoped quantum wells. The lack of a HH1-CB1 exciton, strong temperature dependence of absorption at the Fermi level,

and lack of abnormal temperature dependence of higher subband excitons set apart the FES and are frequently used to identify it in spectroscopic observations.

Additional verification that this observed transition is the FES comes from self-consistently solving the Schrödinger and Poisson equations [39]. This theory uses a 4-band approach taking non-parabolicity into account. The theoretical position of the FES is determined by first using the electron concentration to find $\bar{k}_F$ as in Equation 9-1.

$$\bar{k}_F = \sqrt{2\pi n}$$

Equation 9-1

With this value, the calculated $E - v_s - \bar{k}$ curve is used to determine the energy shift due to the higher Fermi level.

The samples studied for this portion of the research were MBE grown, 250Å multiple quantum wells, with 10 periods. Each sample had an aluminum concentration in the barrier nominally of 9%. They were delta doped with silicon during growth to introduce electrons, raising the Fermi level while minimizing impurity scattering of carriers. A diagram of one such sample is shown in Figure 4-1. The electron concentrations ranged from $n = 1.3 \times 10^{11} \text{ cm}^{-2}$ to $n > 7 \times 10^{11} \text{ cm}^{-2}$ per well. Electron concentration was determined via low magnetic field Hall measurements. All samples were prepared for analysis as described in Chapter 4. Table 9-2 lists sample characteristics.

9.2 Method of Analysis

A series of (ideally) identical multiple quantum well samples with different doping densities were grown to determine effects due to changes in electron concentration. Slight variations in well thickness among samples should yield insignificant spectral differences due to their width (wide wells being less susceptible to small width differences). Similarly, small differences in barrier aluminum concentration in the samples are not expected to have significant effects on lower subbands. These samples were all measured to have an aluminum concentration of 8.7%. Any differences in observations between samples are primarily due to changes in the electron concentration.

Since the temperature dependence of the FES is key to its identification, the method of taking spectra of the same sample over a range of temperatures and calculating a difference spectrum was used in a similar manner to that discussed in earlier chapters. One additional step is required in this analysis due to how the difference spectra are calculated. They are calculated by Equation 9-2:

$$Difference = \frac{T_{Low} - T_{High}}{T_{Low} + T_{High}}$$

Equation 9-2

In this equation, $T_{Low/High}$ stands for the lower/higher temperature spectrum. This essentially means that a 4K-20K plot is normalized differently than a 30K-50K plot. This could yield greatly varying intensities for specific transitions in the same sample, making it difficult to accurately observe temperature dependence of the FES. The

solution to this issue comes from theory. Since transitions involving higher conduction subbands should only show temperature dependence similar to that of undoped wells, the spectra were normalized to the peak of the HH2-CB2 exciton. Any changes in the FES due to temperature are therefore relative to this transition.

The first step in this analysis is to calculate each of the difference spectra per Equation 9-2. Then, each spectrum is shifted by a uniform amount so that each value in the energy range of observed transitions is positive (roughly 250meV to 350meV for 250Å well samples). Noting that there is a local minimum on the high-energy side of the HH2-CB2 exciton, the individual spectra are shifted by the value that places this point at zero on the vertical axis. Finally, they are normalized so that the peak of the HH2-CB2 exciton has a magnitude of one in each case.

Another difference in the analysis of these doped samples as compared to undoped multiple quantum wells is the determination of their Fermi levels. As previously mentioned, the Fermi wave vector is calculated through Equation 9-1. The Microsoft Basic program *Qwkt_d.bas*, listed in Appendix E, is used to calculate the conduction subband dispersion curves based on quantum well parameters (width, aluminum concentration, and offset). Figure 9-4 shows these curves for a 250 Å sample with 9% aluminum in the barrier and an offset of 0.62. The calculated Fermi wave vector for a sample based on an electron concentration of $1.3 \times 10^{11} \text{ cm}^{-2}$ is $\bar{k}_F = 9.04 \times 10^5 \text{ cm}^{-1}$. Identifying this point on the curve for the lowest subband yields a Fermi level of 0.036eV. The minimum of this subband is at 0.0184eV. The

difference in these values gives an estimate for the energy shift from $\bar{k} = 0$ that one would expect to see the FES. In this example, the shift is approximately 18meV. A similar analysis is carried out for each electron concentration. The results are listed in Table 9-3.

9.3 Results

Unless otherwise noted, the results presented in this section are normalized per the above discussion. The temperature dependence of each sample is presented, as are the effects of different electron concentrations in the quantum wells. Figure 9-5 shows the behavior of transitions in S670 ($n=1.3 \times 10^{11} \text{cm}^{-2}$) as temperature is increased. Figure 9-6 is a similar plot of sample S474 ($n=2.4 \times 10^{11} \text{cm}^{-2}$). A clearer view of the plots of S474 is shown in Figure 9-7. The dashed lines track the positions of the HH2-CB2 and FES peaks. The higher temperature FES peaks are difficult to detect in Figure 9-7 because they have greatly decreased in intensity relative to the HH2-CB2 transition. Figure 9-8 more clearly shows that the FES is still detectable in the 77K-110K spectra. The FES is indistinguishable in the 140K-170K spectra (Figure 9-9), which is shown with the 77K-110K spectra for comparison. Figure 9-10 depicts the temperature behavior of sample S669 ($n=3.38 \times 10^{11} \text{cm}^{-2}$). The differences from earlier spectra will be discussed in the next section. The spectra for sample S671, which has a concentration of greater than $7 \times 10^{11} \text{cm}^{-2}$, are presented in Figure 9-11. These spectra were normalized differently due to the lack of a clear HH2-CB2 transition. With these spectra, the peaks of the absorption edge were normalized to

one after the spectra were shifted so that the local minimum on the low energy side of this peak was shifted to zero (the high energy side of the absorption edge was too noisy to pick an unambiguous minimum).

9.4 Discussion

For samples S670 and S474, the FES is clearly apparent from the temperature dependence and shift from the calculated HH1-CB1 position. The clearest results come from S474, in which the Fermi level is well separated in energy from the bottoms of the first and second conduction subband. Figure 9-7 shows the expected decrease in intensity in the FES relative to the HH2-CB2 transition as temperature is increased in S474. The shift to lower energies as temperature is increased is typical of the band gap dependence on temperature discussed in Chapter 6. Comparing the solid lines in Figure 9-7 to Figure 6-5 for the 9% alloy, one sees a relatively constant energy up to approximately 50K, above which the energy drops off at a greater rate. The lines track the progression of the high-energy inflection of the FES and HH2-CB2 peaks with temperature. Interestingly, the FES moves to lower energies at a faster rate than the HH2-CB2 exciton, which shifts by approximately 15meV between 4.2K and the 110K-140K plot (which is the same amount as the 9% data indicates in Figure 6-5). This is likely due – at least in part – to the smearing of the Fermi edge with increasing temperature. Two issues may come into play here. One is an apparent structure, which is discussed next. The other is that the smeared Fermi surface at higher temperatures may cause the FES to interact with the HH2-CB2

exciton. This has been observed and discussed theoretically when the Fermi edge is close in energy to the $n=2$ exciton [53][54].

In S474 and S669, a feature is seen slightly higher in energy than the self-consistently calculated HH1-CB1 subband separation. As the first conduction subband is populated, it cannot be the HH1-CB1 transition, and it is clearly distinguishable from the FES. It exhibits a similar temperature behavior to that of the FES in that the intensity relative to the HH2-CB2 transition decreases as temperature is increased. This may contribute to the greater width of the FES in S670 as compared to S474 since this feature and the predicted FES energy overlap. Figure 9-12 is a plot of the low temperature spectra for these two samples. The arrows mark the predicted FES position for each sample. In S671, which has the highest electron concentration, there is a slight peak at the same position as the feature seen slightly above the $\bar{k} = 0$ position in the other samples, though its strength is barely above the background and no conclusion can be made as to whether it is the same phenomena. The origin of this feature is unexplained at this time and bears further investigation, though that is beyond the scope of this dissertation.

The FES in sample S669 is predicted to occur (Table 9-3) at approximately 310meV. The low temperature measurement (4K-30K) in Figure 9-10 shows a broadening of the HH2-CB2 transition on the low energy side. This is consistent with the occurrence of the FES at this energy. Unlike samples with lower electron concentrations, the HH2-CB2 transition narrows in width as temperature is increased.

This reduction in width is due to changes in line shape on the low energy side of the transition, further supporting the observation that this is the FES.

In sample S671, the electron concentration is great enough to begin filling the second conduction subband. The Fermi level is calculated to be at least 97meV above the bottom of the first subband and at least 34meV above the bottom of the second subband. The spectra for this sample are presented in Figure 9-11. As noted above, these spectra are normalized to the peak of the absorption edge due to the disappearance of the HH2-CB2 exciton. The most notable feature in these spectra is the temperature dependant broadening on the low energy side of the absorption edge. Based on the self-consistently calculated subband spacing in these doped wells, the electron concentration, and the dispersion relation depicted in Figure 9-4, this occurs roughly 50meV above where one would expect to see the FES associated with the first subband and 40meV above where one would expect to see the FES associated with the second subband. The 4K-20K curve is also presented to show that this feature is not due to a greater temperature separation in the difference spectrum. An FES in the second subband would be expected to occur at approximately 350meV. Whether due to the different normalization or other factors, any structure below the absorption edge is too weak too assign to any transition.

9.5 Conclusions

The Fermi Edge Singularity has been observed in the doped $InSb / Al_xIn_{1-x}Sb$ MQW system. Variations with temperature and electron concentration are consistent with

predictions and with its' observation in other material systems. The FES is most clearly observable when the Fermi level is well separated from any subband minima. Some features of the spectra presented in this chapter bear further investigation. First is a feature in the difference spectra occurring at what would be just above calculated the HH1-CB1 subband separation in these wells. Additionally, a detailed study of interactions between the FES and HH2-CB2 exciton as the Fermi level approached the second conduction subband would be interesting. In a moderately doped sample, such that the second subband is populated at a lower level than S671 but higher than S669, an FES associated with this subband may be observed. The issue of how to normalize these spectra should be resolved prior to doing this experiment. A final issue worth investigating is the shift in position of the HH2-CB2 exciton with changes in electron concentration, especially since the shift is not monotonic. The observed HH2-CB2 transition energies are listed in Table 9-4. As the aluminum concentrations are the same for each crystal (as verified via the method presented in Chapter 6), barrier height cannot account for this. Additionally, calculations show that well thickness between samples would have to differ by roughly 20Å – or nearly 10% - to account for these shifts, which is unlikely based on the consistency in aluminum concentration and the experience of the growers. While this chapter has only touched on some of the general aspects of the Fermi Edge Singularity, it is a subject worthy of further research, both experimental and theoretical.

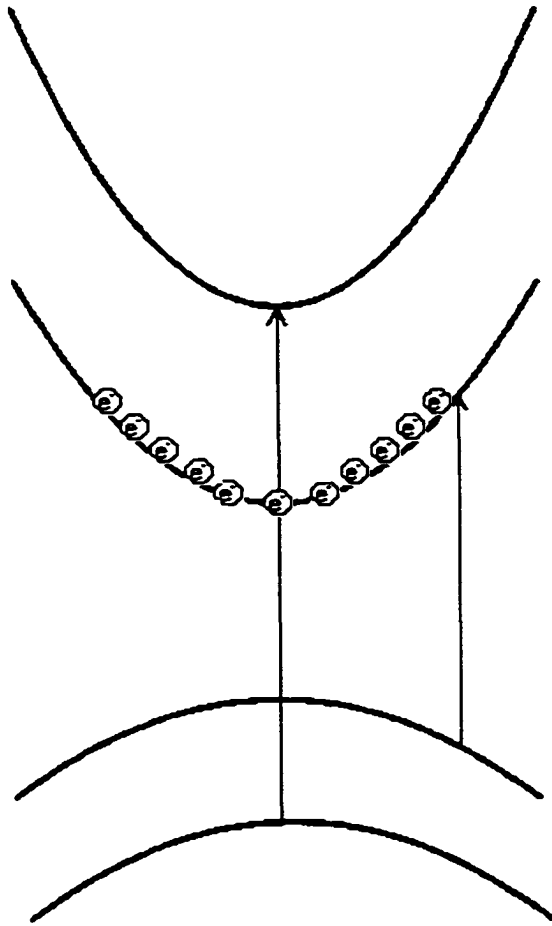


Figure 9-1 Depiction of Fermi Edge Transition

Direct transitions from the first valence subband can only occur at the Fermi Level since all lower conduction subband states are filled. Higher subband transitions can occur at $k=0$ since higher conduction subband states are not filled.

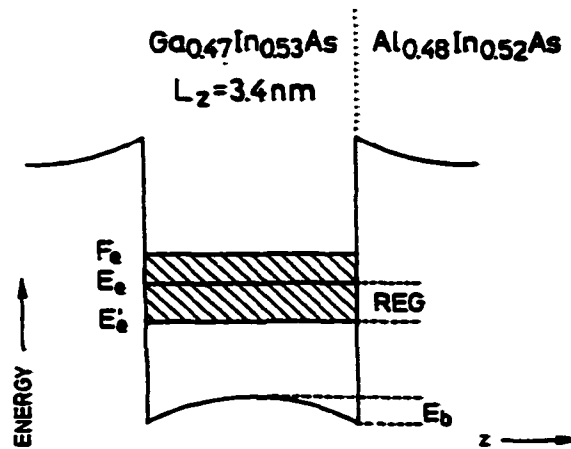


Figure 9-2 Effects of Charge on Potential Profile

The curvature in the band profile is due to the electrostatic potential of ionized donors in the barrier and the excess electrons in the well [51].

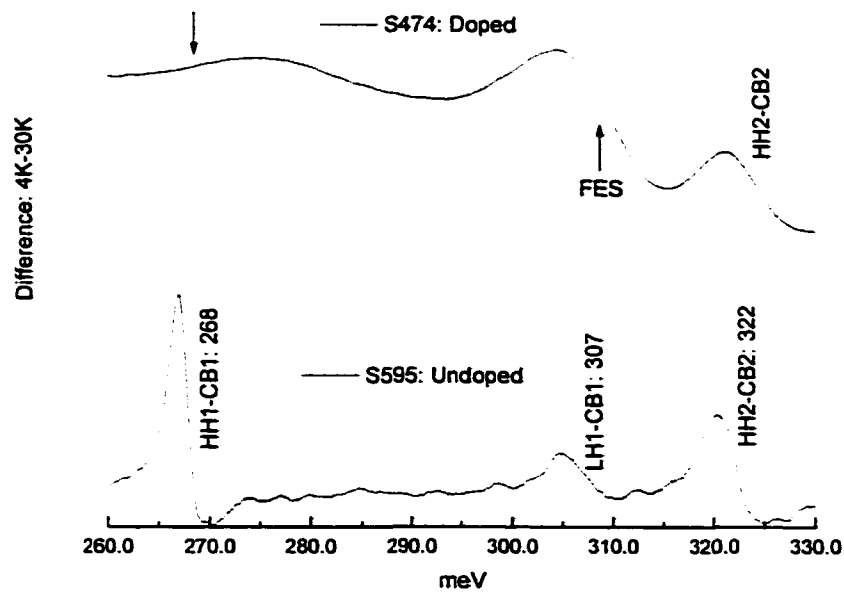


Figure 9-3 Difference Spectra of an Undoped and a Doped 250Å MQW

The effect of doping is seen in sample S474, which is otherwise identical to sample S595. The left arrow on the curve for S474 depicts where the HH1-CB1 transition occurs in the undoped S595.

Table 9-1 Self-Consistently Calculated Subband Separation

$n(\times 10^{11} \text{ cm}^{-2})$	HH1-CB1 (eV)	HH2-CB2 (eV)
undoped	0.269	0.321
1.3	0.27	0.322
2.4	0.2714	0.325
3.38	0.272	0.326
7		0.322

Table 9-2 Doped Sample Parameters

Sample	Well Width	Barrier Aluminum Concentration	$n (\text{cm}^{-2})$
S670	250Å	0.087	1.3×10^{11}
S474	250Å	0.087	2.4×10^{11}
S669	250Å	0.087	3.38×10^{11}
S671	250Å	0.087	$> 7 \times 10^{11}$

Subbands

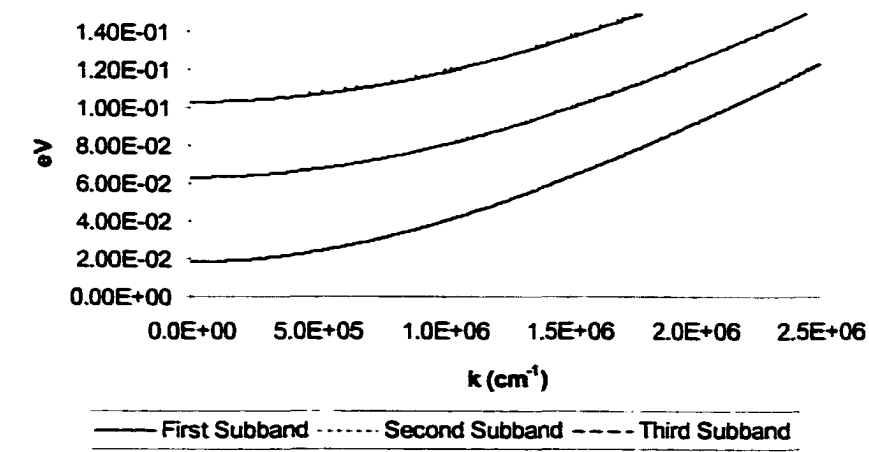


Figure 9-4 Calculated Conduction Subband Dispersion Relations

These numerically calculated curves are for the conduction subbands in a 250Å quantum well with barrier aluminum concentration of 9%. The previously determined value of 0.62 for band offset is used in these calculations.

Table 9-3 Concentration and Predicted Shift of FES

$n \text{ (cm}^{-2}\text{)}$	$k_{\text{Fermi}} \text{ (cm}^{-1}\text{)}$	$E_{\text{Fermi}} \text{ (eV)}$	Shift (eV)
1.3×10^{11}	9.04×10^5	3.6×10^{-2}	.018
2.4×10^{11}	1.23×10^6	4.96×10^{-2}	.0312
3.38×10^{11}	1.46×10^6	6.08×10^{-2}	.0424
7×10^{11}	2.1×10^6	9.73×10^{-2}	.0337*

*Note that in this case, the energy shift is with respect to the bottom of the second subband.

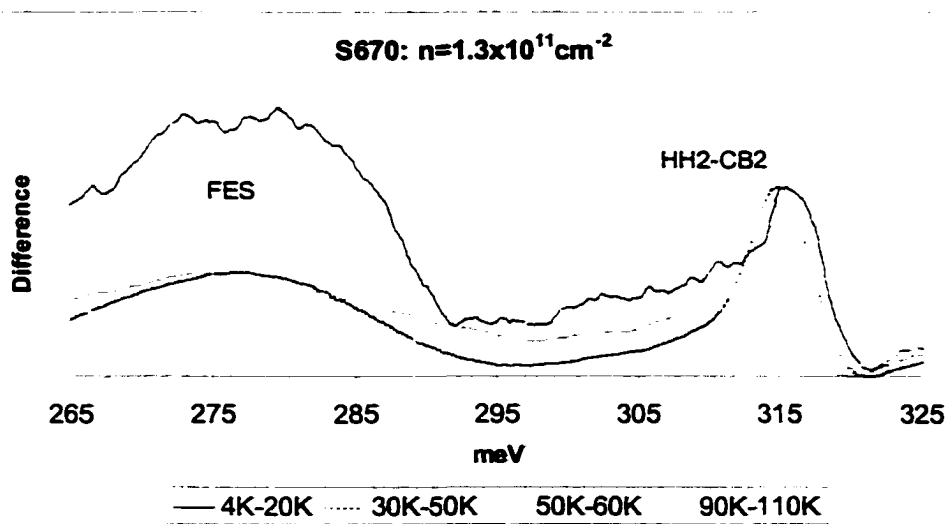


Figure 9-5 Difference Spectra of S670

The weakening of the Fermi Edge Singularity with increasing temperature is seen in this set of spectra of sample S670.

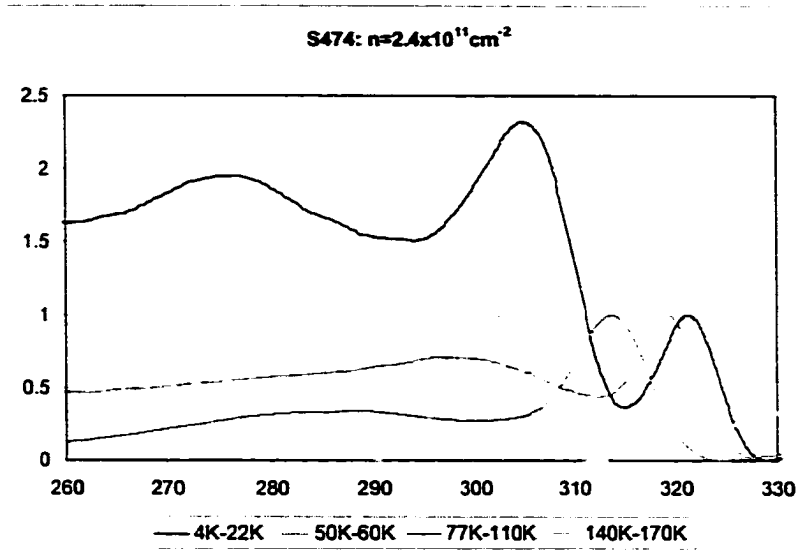


Figure 9-6 Difference Spectra of S474

The temperature dependence of the FES is seen in sample S474.

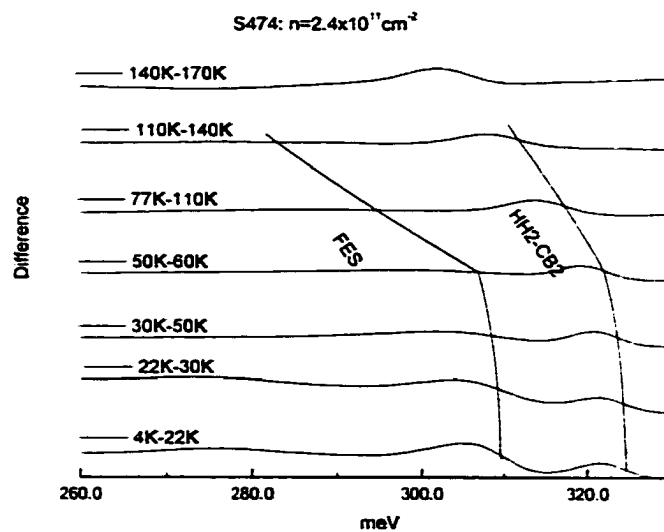


Figure 9-7 Temperature Dependence of FES in S474

The FES and HH2-CB2 exciton shift to lower energy as temperature is increased. The solid lines labeled FES and HH2-CB2 track this shift with temperature.

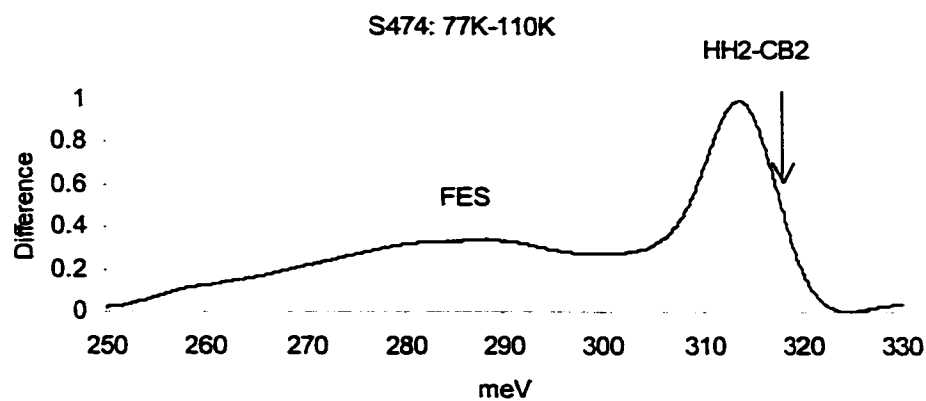


Figure 9-8 77K-110K Spectrum of S474

The FES is still clearly present in sample S474 up to approximately 100K.

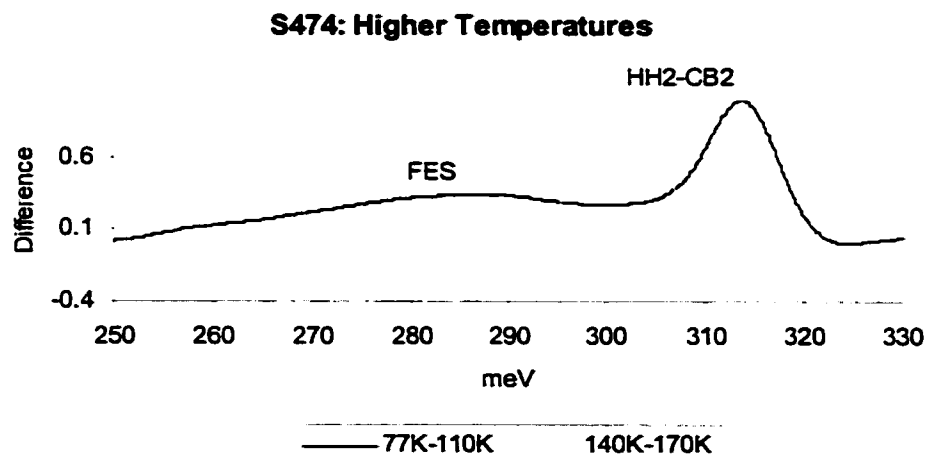


Figure 9-9 S474 at Higher Temperatures

Above 140K, no evidence of the FES can be seen in sample S474.

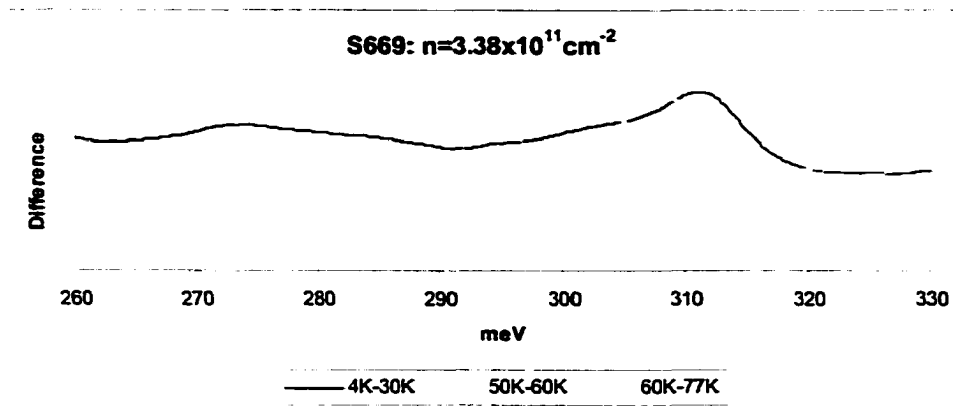


Figure 9-10 Temperature Dependence in S669

These spectra are normalized to the HH2-CB2 transition (the high points on the curves near 310meV). The low energy broadening of the HH2-CB2 transition in the 4K-30K - and its reduction in the higher temperature curves - is consistent with the predicted position of the FES and its temperature dependence.

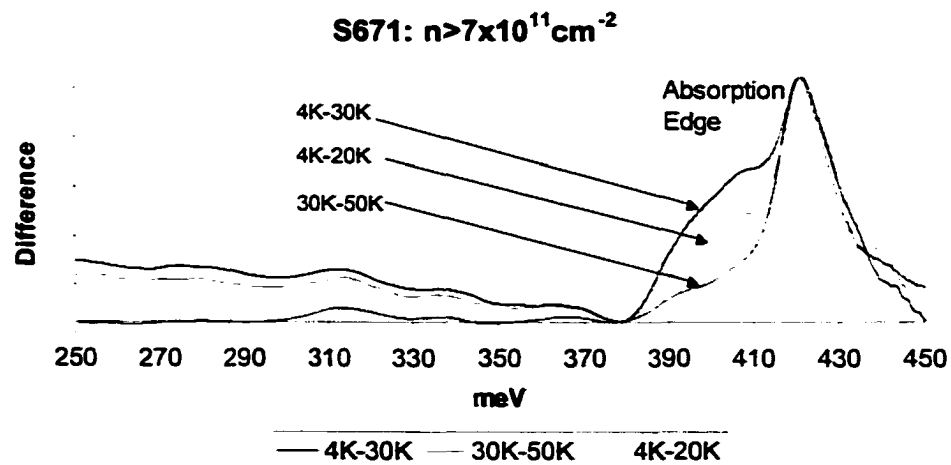


Figure 9-11 Temperature Dependence in S671

Spectra for sample S671 were normalized to the absorption edge as no HH2-CB2 was observed due to the high electron concentration.

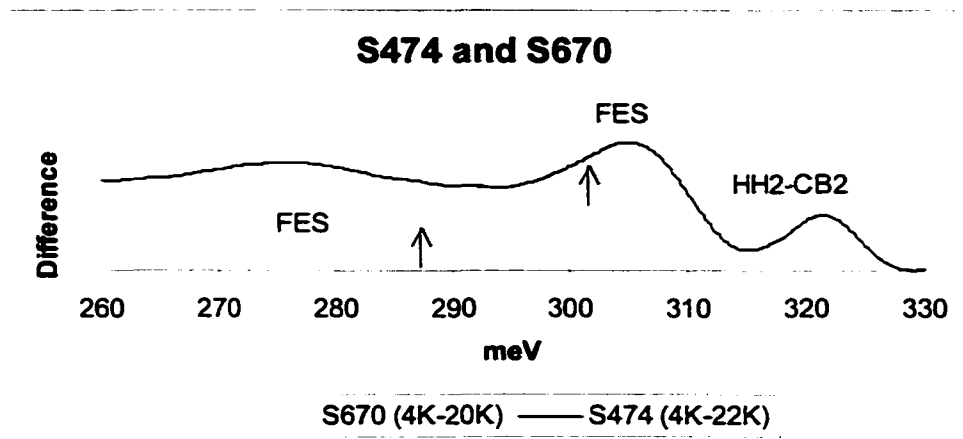


Figure 9-12 Comparison of S474 and S670

The predicted positions of the FES is marked with an arrow in each curve. The higher electron concentration of sample S474 has shifted the FES to higher energy than that in sample S670.

Table 9-4 HH2-CB2 Transition Energies

Sample	$n \text{ (} \times 10^{11} \text{ cm}^{-2} \text{)}$	Energy (meV)
undoped	0	322
s670	1.3	318.5
s474	2.4	325.4
s669	3.38	315.1

Chapter 10: Conclusions

This research has led to a progressively better understanding of the properties of the $InSb/Al_xIn_{1-x}Sb$. One result of Chapter 6, a simple relationship between absorption edge and aluminum concentration, has proven invaluable in subsequent portions of this research and can be of equal use to those who continue to investigate this material system. Examination of the band gap temperature dependence – a fundamental finding of this research – has practical results in terms of this research. It is a justification of the technique of taking a difference spectrum, as well as a means of determining its limits. Determining of the $InSb/Al_xIn_{1-x}Sb$ band offset has been essential in evaluating models that help understand observations. Additionally, it is directly related to the ability to engineer $InSb/Al_xIn_{1-x}Sb$ devices. The work on deformation potentials, though incomplete to date, has led to a method of analysis that the author believes to be valuable. Observation of the Fermi Edge Singularity in doped $InSb/Al_xIn_{1-x}Sb$ quantum wells yields data that can lead to a better theoretical model of band structure and the many body physics of a Fermi gas. Further research opportunities include luminescent studies of doped and undoped quantum wells, the study of magneto-excitons, and the examination of intersubband transitions in doped samples. It is the hope of this author that this work assists others in their research.

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Appendix A. Beam Splitter Manual Alignment

IMPORTANT: The manufacturer recommends against this procedure, however it has needed to be done on new beam splitters from them. Undertake these steps with care and patience, and as a last resort. Usually, errors due to alignment can be fixed by running “Auto Align”.

1. Turn power to spectrometer off.
2. Open top electrical compartment.
3. Connect oscilloscopes to leads A, B, and R from Pin J290 (to the left of the A/D converter). This reads output from the laser detectors.
4. Close top electrical compartment.
5. Open mail chamber.
6. Disconnect power cord P223. This drives the piezoelectric alignment of the beam splitter.
7. Turn on spectrometer.
8. Turn on oscilloscopes.
 - a. Comment: The goal is to simultaneously maximize the three sine curves on the oscilloscopes to 10 volts. The beam splitter has three

allen screws (3/32 inch). These are adjusted for aligning the beam splitter.

9. Firmly grasp the beam splitter handle. Gently press forward, then backward.

Twist clockwise and then counterclockwise. Observe which of these motions increases all the signals to the oscilloscopes.

10. Take beam splitter out of the holder, only handling the frame. If signal strength increases in the forward direction (towards the piezo connectors), then adjust the bottom screw by turning clockwise. This example is given as a reference. The direction may need to be different depending on whether the increase is due to a backward motion or a twist. The amount of the turn needs to be almost imperceptible or you will likely overshoot your goal.

11. Put the beam splitter back in the spectrometer and observe the curves.

12. Steps 9–11 may need to be repeated a number of times to achieve adequate alignment. Small improvements each time are the best way to not mess up the alignment more.

13. Ideally, one motion will increase all three traces. If not, find the adjustment that increased two or one of them.

- a. Comment: A slight increase in two traces is better than a large increase in just one trace.
14. Having maximized one or two of the traces, repeat steps 9-11 again to increase the third trace. Some drop in voltage of the first two traces is acceptable. After increasing the voltage of the third trace, repeat steps 9-11 again.
15. Once the above steps are complete (or if they are unsuccessful), one needs to turn off the moving mirror. This is accomplished by opening the OBE compartment on the left side of the spectrometer and flipping the Coil switch to off.
16. Place a strip of white paper in front of the three laser detectors so that the laser interference pattern can be observed.
 - a. The goal here will be to maximize the size of the interference fringes through rotating the beam splitter as described in step 9.
17. Turn off the room lights.
18. Observe which motion increases the size of the fringes. If the beam splitter is near to alignment, the fringes will begin to form a circular pattern on the strip of paper. Try to get the central fringe (or close to it) over the laser detectors.

19. Make adjustments to the allen screws as in step 10.

- a. Comment: This method using the laser interference fringes can often be used to increase signal strength, even if the beam splitter appears to be aligned. This is definitely a fine-tuning adjustment.

Appendix B. Parameter File

APT=OPEN
APTYP=TRIANG
BACK=
BANDEDGE1=0.2
BANDEDGE2=0.8
BEAM=INT
BGREG=DEFAULT
BIDIR=Y
CMPRES=FULL
CMPTO=ABS
CSIGNAL=AUTO
DAPTYP=TRIANG
DELAY=3.0
DET=INT1
DNSPEC=10
DSPCOLOR=DIFFERENT
DSPMOVE=TOGETHER
DSPOFFSET=NONE
ELWN=15800.8235
ENP=6000.0
ESCBEAM=INT
FFP=1000.0
FGREG=/usr/lib/fgreg
FILTER=5
FLP=6000.0
FLTRTYP=HP

GCDELAY=0
GCNBACK=20
GCNBASIS=20
GCTIME=45
GRDATA=/usr/lib/kin/GRDATA
GRR=400
GSREG=DEFAULT
HWIDTH=10.0
IFREQ=AUTO
INTFACT=1
INTG=NO
ISCA=Y
KCOMPREG=ALL
KCMPSPEC=KSPEC
KMBASE=AUTO
KVAL=2.0
LEFT=500.0
MENCOL=740b80b00b00f
MICRONRES=0.2
MORE=N
NEWSPEC=trans
NLV=0.05
NPOINTS=AUTO
NSAMPS=3
OBEZTEST=0
ORDER=2
ORIENT=NORMAL
PAPERSIZ=SM

PAXES=Y

PCOMM= spectrum of InSb QW on GaAs

PEN=AUTO

PKSENS=I

PKSOURCE=G/S

PKTAB=Y

PLABEL=InSb PLOTPAGE=Y

PLOTTER=AUTO

PLUNITS=CM

PMAMP=0.0

PMFREQ=400HZ

PPARMS=RES, BACK, SCANS, FILTER, SPEED, SEN

PSDESC=

PXOFF=AUTO

PYOFF=AUTO

RC=BOTH

REF=77k

RES=4

RIGHT=00.0

RTDMON=NO

RUNCOMMENT=

RUNTITLE=

SAMP=rtt54t

SAMP10=

SAMP2=01104a02

SAMP3=01104a03

SAMP4=

SAMP5=

SAMP6=
SAMP7=
SAMP8=
SAMP9=
SCANS=64
SCANTO=SB
SCBACK=1.000
SCNSTOR=256
SCSAMP=1.000
SEN=3
SIGNAL=AUTO
SOURCE=SRC1
SPECN=1
SPEED=20
SSP=NO
STDELAY=AUTO
STP=1000.0
SUBFAC=1.0
SUBTYPE=H2O
SUMAX=AUTO
SUMIN=AUTO
SVIG=Y
SVIM=N
SVMR=N
SVSB=Y
SYM=asym
TRANSBW=0.05
TRSRES=10.0us

TRSWIDTH=100

UDR=2

XSB=0

XSCALE=100

XSIZE=AUTO

YMAX=AUTO

YMIN=AUTO

YSCALE=100

YSIZE=AUTO

ZFF=2

Appendix C. Scripts

C.1. *Script: asci*

: This script converts IDRIS .dt and .ig files to ascii

: Say you have files data.dt and data.ig and want to

: convert them to ascii files. Use the syntax below:

: asci data

: The script will take care of the extensions.

```
cp $1.dt temp.dt
```

```
dtDump2 temp.dt > $1.dat
```

```
rm temp.dt
```

```
: rm temp.IG
```

C.2. Script: convert

`asci 01119a02`

`asci 01119a03`

`asci 01119a04`

`asci 01119a01`

Note that the “convert” script calls the “asci” script with filenames to of data one wishes to convert.

Appendix D. Deformation Potential Program and Input File

D.1. Fit.cpp

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <time.h>

// Declarations for Drand48.c
double drand48();
void srand48(long seedval);

# define pi 3.14159265358979323846
# define INFILE "samples.in"
# define OUTFILE "eval.out"
# define STATFILE "stat.out"
//# define x 0.275 // Al Concentration
# define m0 9.10956e-28 // electron bare mass g
# define ev 1.60219e-19 // lev=1.60219E-19 J
# define a1 6.46955e-8 //strain coeff.
# define a3 6.12814e-8
# define a2 (a1*(1.0-x[h])+a3*x[h])
# define st ((a2-a1)/a1)
# define vd 0.0
# define hb 1.05459e-27
# define cf 1.60219e-12 // Factor to change the unit to cgs
# define delw 0.81 // eV delta value for well
# define delAlSb 0.676 // eV delta value for AlSb
# define de 0.0002 // Energy interval in eV
# define p sqrt(11.3*cf/m0) // Coupling factor
# define band_offset 0.62 // Fractional band offset

# define MAX_SAMPLES 100
# define FULL_EXPRESSION 1

// --- BEGIN Subroutines -----

// Read parameters from file
void
read_params (char *filename, double *a, double *b, double *Eq,
             double *ML, int *stat_iterations, int *gap_feedback)
{
    FILE *infile;
    char lbuff[256];
    int i, cc;

    printf ("Reading parameters from %s\n", filename);
    infile = fopen (filename, "r");
    if (infile == NULL) {
        printf ("Couldn't open parameter file. Skipping...\n");
        return;
    }
}
```

```

while (!feof (infile)) {
    if (fgets (lbuff, sizeof (lbuff), infile) == NULL)
        break;
    // compress whitespace in input line
    cc = 0;
    for (i = 0; (lbuff[i] != '\000') && (i < sizeof (lbuff)); i++) {
        if ((lbuff[i] != ' ') && (lbuff[i] != '\t') && (lbuff[i] != '\n')) {
            lbuff[cc] = lbuff[i];
            cc++;
        }
    }
    lbuff[cc] = '\000';
    if (lbuff[0] == '#')
        continue;
    if (strcmp ("data", lbuff) == 0)
        break;
    i = 0;
    while ((lbuff[i] != '=') && (lbuff[i] != '\000'))
        i++;
    if (lbuff[i] == '=') {
        lbuff[i] = '\000';
        i++;
    }
    else {
        printf ("Bad configuration line: %s\n", lbuff);
        continue;
    }
    if (strcmp ("a", lbuff) == 0) {
        sscanf (lbuff + 1, "%lf", a);
    }
    else if (strcmp ("b", lbuff) == 0) {
        sscanf (lbuff + 1, "%lf", b);
    }
    else if (strcmp ("ML", lbuff) == 0) {
        sscanf (lbuff + 1, "%lf", ML);
    }
    else if (strcmp ("Eg", lbuff) == 0) {
        sscanf (lbuff + 1, "%lf", Eg);
    }
    else if (strcmp ("StatIterations", lbuff) == 0) {
        sscanf (lbuff + 1, "%d", stat_iterations);
    }
    else if (strcmp ("GapFeedback", lbuff) == 0) {
        sscanf (lbuff + 1, "%d", gap_feedback);
    }
    else {
        printf ("Unknown parameter: \"%s\"\n", lbuff);
    }
}
fclose (infile);
}

// Read data from file
int
read_data (char *filename, double *x, double *hh, double *lh,
           double *hh_stat_weight, double *lh_stat_weight,
           double *hh_err, double *lh_err, int max_data)
{
    int count, nvals;
    char s1[256], s2[256], s3[256], s4[256], s5[256];
    char lbuff[256];

```

```

FILE *infile;
double x_conc, hh_energy, lh_energy;
int i, cc;

infile = fopen (filename, "r");

count = 0;
while (!feof (infile)) {
    if (fgets (lbuff, sizeof (lbuff), infile) == NULL)
        break;
    cc = 0;
    for (i = 0; (lbuff[i] != '\000') && (i < sizeof (lbuff)); i++) {
        if ((lbuff[i] != ' ') && (lbuff[i] != '\t') && (lbuff[i] != '\n')) {
            lbuff[cc] = lbuff[i];
            cc++;
        }
    }
    lbuff[cc] = '\000';
    if (strcmp ("data", lbuff) == 0)
        break;
}

while ((!feof (infile)) && (count < max_data)) {
    if (fgets (lbuff, sizeof (lbuff), infile) == NULL)
        break;
    nvals = sscanf (lbuff, "%s %s %s %s %s", s1, s2, s3, s4, s5);
    sscanf (s1, "%lf", &x_conc);
    if (strcmp (s2, "NA") == 0) {
        hh_energy = 0.0;
        hh_stat_weight[count] = 0.0;
    }
    else {
        sscanf (s2, "%lf", &hh_energy);
        hh_stat_weight[count] = 1.0;
    }
    if (strcmp (s3, "NA") == 0) {
        lh_energy = 0.0;
        lh_stat_weight[count] = 0.0;
    }
    else {
        sscanf (s3, "%lf", &lh_energy);
        lh_stat_weight[count] = 1.0;
    }
    if (nvals == 5) {
        if (strcmp (s4, "NA") == 0) {
            hh_err[count] = 0.0;
        }
        else {
            sscanf (s4, "%lf", &(hh_err[count]));
        }
        if (strcmp (s5, "NA") == 0) {
            lh_err[count] = 0.0;
        }
        else {
            sscanf (s5, "%lf", &(lh_err[count]));
        }
    }
    else {
        lh_err[count] = 0.0;
        hh_err[count] = 0.0;
    }
    x[count] = x_conc;
    hh[count] = hh_energy;
    lh[count] = lh_energy;
}

```

```

        count++;
    }
    fclose (infile);
    return count;
}

// Linear least squares
void
linear_least_squares (double *x, double *y, double *stat_weight, int n,
                      double *slope, double *intercept)
{
    int i;
    double Sx, Sy, Sxx, Sxy, SSxx, SSxy, W_sum;

    Sx = Sy = Sxx = Sxy = W_sum = 0.0;
    for (i = 0; i < n; i++) {
        Sx += x[i] * stat_weight[i];
        Sy += y[i] * stat_weight[i];
        Sxx += x[i] * x[i] * stat_weight[i];
        Sxy += x[i] * y[i] * stat_weight[i];
        W_sum += stat_weight[i];
    }

    SSxy = Sxy - (Sx * Sy) / W_sum;
    SSxx = Sxx - (Sx * Sx) / W_sum;

    *slope = SSxy / SSxx;
    *intercept = (Sy - *slope * Sx) / W_sum;
    // printf("Stats : %lf %lf %lf %lf Weight=%lf\n",Sx,Sy,SSxx,SSxy,W_sum);
}

double
d_sign (double x)
{
    if (x < 0.0)
        return -1.0;
    else if (x == 0.0)
        return 0.0;
    else
        return 1.0;
}

// A dual linear least squares fit with shared intercept
void
dual_linear_least_squares (double *x1, double *y1, double *stat_weight1,
                           int n1, double *x2, double *y2,
                           double *stat_weight2, int n2, double *slope1,
                           double *slope2, double *intercept)
{
    int i;
    double Sx1, Sy1, Sxx1, Sxy1, W_sum1;
    double Sx2, Sy2, Sxx2, Sxy2, W_sum2;

    Sx1 = Sy1 = Sxx1 = Sxy1 = W_sum1 = 0.0;
    Sx2 = Sy2 = Sxx2 = Sxy2 = W_sum2 = 0.0;

    for (i = 0; i < n1; i++) {
        Sx1 += x1[i] * stat_weight1[i];
        Sy1 += y1[i] * stat_weight1[i];
        Sxx1 += x1[i] * x1[i] * stat_weight1[i];
        Sxy1 += x1[i] * y1[i] * stat_weight1[i];
    }

```

```

    W_sum1 += stat_weight1[i];
}

for (i = 0; i < n2; i++) {
    Sx2 += x2[i] * stat_weight2[i];
    Sy2 += y2[i] * stat_weight2[i];
    Sxx2 += x2[i] * x2[i] * stat_weight2[i];
    Sxy2 += x2[i] * y2[i] * stat_weight2[i];
    W_sum2 += stat_weight2[i];
}

*intercept = (Sy1 - Sy2 - Sx1 * Sxy1 / Sxx1 - Sx2 * Sxy2 / Sxx2) /
    (W_sum1 + W_sum2 - Sx1 * Sx1 / Sxx1 - Sx2 * Sx2 / Sxx2);

*slope1 = (Sxy1 - Sx1 * (*intercept)) / Sxx1;
*slope2 = (Sxy2 - Sx2 * (*intercept)) / Sxx2;
}

// Egw_lh=(Eg_InSb+(a*(2.0-2.0*0.548)+b*(1.0+2.0*0.548))*st
// -(9.0*cf/(4.0*delw))*b*b*(1.0+2.0*0.548)*(1.0+2.0*0.548)*st*st)*cf;
// Egw_lh=(Eg_InSb+a*(2.0-2.0*0.548)*st
// -(delw/2)*(1-(-b)*(1.0+2.0*0.548)*st/delw)
// -(delw/2)*sqrt((1+2*(-b)*(1.0+2.0*0.548)*st/delw)
// +9*(-b)*(1.0+2.0*0.548)*st/delw)*((-b)*(1.0+2.0*0.548)*st/delw)
// ))*cf;

// Calculate LH-HH function for b, x
void
calc_func (double *pars, double x, double *val, double *grd)
{
    double b, Eg0, g1, g2, btrm;

    // Now has lh-hh expression
    g1 = (2.0 - 2.0 * 0.548);
    g2 = (1.0 + 2.0 * 0.548);
    b = pars[0];
    btrm =
        1.0 - 2.0 * g2 * b * x / delw +
        9 * g2 * g2 * b * b * x * x / (delw * delw);

    *val = (0.5 * delw) + 1.5 * g2 * b * x - (0.5 * delw) * sqrt (btrm);
    grd[0] =
        1.5 * g2 * x - 0.5 * (-g2 * x +
        9 * g2 * g2 * b * x * x / delw) / sqrt (btrm);
}

// Calculate Chi^2, alpha and beta matrices for Levenberg-Marquardt
void
calc_mats (double *pm, int nv, double *x, double *y, double *wt, int n,
    double *chi2, double *alpha, double *beta)
{
    int i, j, k;
    double v, df, *grd;

    grd = (double *) malloc (nv * sizeof (double));

    *chi2 = 0.0;
    for (i = 0; i < nv; i++)
        beta[i] = 0.0;
    for (i = 0; i < nv * nv; i++)
        alpha[i] = 0.0;

    for (i = 0; i < n; i++) {
        calc_func (pm, x[i], &v, grd);
    }
}

```

```

        df = y[i] - v;
        *chi2 += df * df * wt[i];
        for (j = 0; j < nv; j++) {
            beta[j] += df * grd[j] * wt[i];
            for (k = 0; k < nv; k++)
                alpha[nv * j + k] += grd[j] * grd[k] * wt[i];
        }
    }
    free (grd);
}

// Calculate chi^2
double
calc_chi2 (double *pm, int nv, double *x, double *y, double *wt, int n)
{
    int i;
    double v, df, chi2, *grd;

    grd = (double *) malloc (nv * sizeof (double));
    chi2 = 0.0;
    for (i = 0; i < n; i++) {
        calc_func (pm, x[i], &v, grd);
        df = y[i] - v;
        chi2 += df * df * wt[i];
    }
    free (grd);
    return chi2;
}

// Solve matrix -- very simple gauss
void
solv_mat (double *mat, double *vec, int n, double *x)
{
    int i, j, k;
    double *m, piv;

    m = (double *) malloc (n * n * sizeof (double));
    for (i = 0; i < n * n; i++)
        m[i] = mat[i];
    for (i = 0; i < n; i++)
        x[i] = vec[i];

    for (i = 0; i < n; i++) {
        piv = 1.0 / m[i * n + i];
        for (j = 0; j < n; j++)
            m[i * n + j] *= piv;
        x[i] *= piv;
        for (j = i + 1; j < n; j++) {
            piv = m[j * n + i];
            for (k = 0; k < n; k++)
                m[j * n + k] -= m[i * n + k] * piv;
            x[j] -= x[i] * piv;
        }
    }
    // Back sub
    for (i = n - 2; i >= 0; i--) {
        for (j = n - 1; j > i; j--)
            x[i] -= x[j] * m[i * n + j];
    }
    free (m);
}

// Levenberg-Marquardt non-linear least squares

```

```

void
levmar (double *pm, int nv, double *x, double *y, double *wt, int n)
{
    int i;
    double *alpha, *beta, *alphap, *da, *pt, chi2, ochi2, lambda;

    alpha = (double *) malloc (nv * nv * sizeof (double));
    alphap = (double *) malloc (nv * nv * sizeof (double));
    beta = (double *) malloc (nv * sizeof (double));
    da = (double *) malloc (nv * sizeof (double));
    pt = (double *) malloc (nv * sizeof (double));
    lambda = 0.001;

    // First try is from incoming values

    for (i = 0; i < nv; i++)
        pt[i] = pm[i];
    calc_mats (pm, nv, x, y, wt, n, &chi2, alpha, beta);
    ochi2 = chi2;

    while (1) {
        for (i = 0; i < nv * nv; i++)
            alphap[i] = alpha[i];
        for (i = 0; i < nv; i++)
            alphap[i * nv + i] *= (1.0 + lambda);
        solv_mat (alphap, beta, nv, da);
        for (i = 0; i < nv; i++)
            printf ("%le ", da[i]);
        printf ("\n");
        for (i = 0; i < nv; i++)
            pt[i] = pm[i] + da[i];
        chi2 = calc_chi2 (pt, nv, x, y, wt, n);
        if ((ochi2 - chi2) / chi2 < .000001) {
            for (i = 0; i < nv; i++)
                pm[i] = pt[i];
            break;
        }
        printf ("Chi2= %le Old= %le\n", chi2, ochi2);
        if (chi2 < ochi2) {
            for (i = 0; i < nv; i++)
                pm[i] = pt[i];
            calc_mats (pm, nv, x, y, wt, n, &chi2, alpha, beta);
            lambda *= 0.1;
        }
        else {
            lambda *= 10;
        }
        ochi2 = chi2;
        printf ("Vec:");
        for (i = 0; i < nv; i++)
            printf ("%le ", pm[i]);
        printf ("\n");
        printf ("Chi2= %le lambda=%le\n", chi2, lambda);
    }

    free (pt);
    free (da);
    free (beta);
    free (alphap);
    free (alpha);
}

// Non-linear least squares

```

```

void
nonlin_fit (double *x, double *y, double *stat_weight, int n, double *b)
{
    double pm[1];

    pm[0] = *b;
    levmar (pm, 1, x, y, stat_weight, n);
    *b = pm[0];
}

double
refine_E (double Egw, double Egb,
          double Vs, double Vp,
          double delB, double wellww,
          double Estart, double Eend,
          double val_hi, double val_lo, int mass_method)
{
    double E, kw, kba, mw, mb, sig, temp, temp1;
    double E_hi, E_lo, v_hi, v_lo, etol;

    E_hi = Eend;
    E_lo = Estart;
    v_hi = val_hi;
    v_lo = val_lo;
    E = 0.5 * (E_hi + E_lo);
    etol = 0.00001 * fabs (Eend - Estart);

    while (fabs (E_hi - E_lo) > etol) {
        if (mass_method == 1) {
            kw =
                sqrt (E * (E + Egw) * (E + Egw + delw * cf) /
                    (E + Egw + (2.0 * delw * cf / 3.0))); / (hb * p);
            kba =
                sqrt ((Vs - E) * (E - Vs + Egb) * (E - Vs + Egb + delB) /
                    (E - Vs + Egb + 2.0 * delB / 3.0))
                / (hb * p);
            mw = 1.0 / ((2.0 / (E + Egw)) + (1.0 / (E + Egw + delw * cf)));
            mb = 1.0 / ((2.0 / (E + Egb - Vs)) + (1.0 / (E + Egb + delB)));
        }
        else {
            mw = 0.24 * m0; // Heavy Hole mass: Based on Luttinger
            mb = Egb * mw / Egw; // Parameters for dispersion mass
            kw = sqrt (-2.0 * mw * (Egw + E)) / hb;
            kba = sqrt (-2.0 * mb * (Egw + E + Vp)) / hb;
        }
        sig = (mb * kw) / (mw * kba);
        temp =
            cos (kw * wellww) - 0.5 * (sig - 1.0 / sig) * sin (kw * wellww);
        if (d_sign (temp) == d_sign (v_lo)) {
            v_lo = temp;
            E_lo = E;
        }
        else {
            v_hi = temp;
            E_hi = E;
        }
        E = 0.5 * (E_hi + E_lo);
    }
    return E;
}

```



```

}

// The Energy Solver
int
e_solver (double Egw, double Egb,
          double Vs, double Vp,
          double delB, double wellww,
          double Estart, double Eend, double dE,
          int mass_method, double *E_sol)
{
    double E, kw, kba, mw, mb, sig, temp, templ;
    int j, k;

    // printf("%le %le %le %le\n",Egw,Egb,Vs,Vp);
    // printf("%le %le %le %le\n",delB,wellww,Estart,Eend);

    E = Estart;
    k = 0;
    temp = templ = 1.0;
    for (j = 0; j < 1000000; j++) {
        E += dE;
        // printf("J=%d, E=%le, dE=%le\n",j,E,dE);
        if (E * dE >= Eend * dE)
            break;

        if (mass_method == 1) {
            kw =
                sqrt (E * (E + Egw) * (E + Egw + delw * cf) /
                      (E + Egw + (2.0 * delw * cf / 3.0))) / (hb * p);
            if (kw < 0) {
                printf ("The well wave vector is negative\n");
                break;
            }
            kba =
                sqrt ((Vs - E) * (E - Vs + Egb) * (E - Vs + Egb + delB) /
                      (E - Vs + Egb + 2.0 * delB / 3.0)) /
                (hb * p);
            if (kba < 0) {
                printf ("The barrier wave vector is negative\n");
                break;
            }
            mw = 1.0 / ((2.0 / (E + Egw)) + (1.0 / (E + Egw + delw * cf)));
            mb = 1.0 / ((2.0 / (E + Egb - Vs)) + (1.0 / (E - Egb - delB)));
        }
        else {
            mw = 0.24 * m0; // Heavy Hole mass: Based on Luttinger
            mb = Egb * mw / Egw; // Parameters for dispersion mass
            kw = sqrt (-2.0 * mw * (Egw + E)) / hb;
            kba = sqrt (-2.0 * mb * (Egw + E + Vp)) / hb;
        }
        sig = (mb * kw) / (mw * kba);
        temp =
            cos (kw * wellww) - 0.5 * (sig - 1.0 / sig) * sin (kw * wellww);
        if ((j > 0) && (d_sign (temp) != d_sign (templ))) {
            E = refine_E (Egw, Egb, Vs, Vp, delB, wellww, E - dE, E,
                          temp, templ, mass_method);
            E_sol[k] = E;
            k++;
            printf ("Energy = %le %lf\n", E, E / cf);
        }
        templ = temp;
    }
}

```

```

// printf("Max J=%d    Final Energy %le\n",j,E);
// printf ("Vp= %le , Egw= %le\n",Vp,Egw);
return k;
}

double
randgauss (double sig)
{
    double u1, u2, z, zz;
    while (1) {
        u1 = drand48 ();
        u2 = drand48 ();
        z = 1.71552776992141 * (u1 - .5) / u2;
        zz = 0.25 * z * z;
        if (zz <= -log (u2))
            break;
    }
    return (sig * z);
}

// --- END Subroutines -----

// .....
// Program to calculate the subband energy for electrons,HH,LH
// For InSb/AlInSb/ Using Bastard 4-band model,kt=0
// .....
// Egw= The well band gap
// Egb= The Barrier band gap
// x= The Al concentration
// vs= Gamma6 band offset
// vp= Gamma8 band offset
// vd= Spin-Orbit band offset
// p= Kane model coupling factor
// delw=Split off band energy in the well
// delb=Split off band energy in the barrier
// Ei[0]= The initial guess for conduction band
// Ei[1]= The initial guess for light hole band
// Ei[2]= The initial guess for heavy hole band
// de=Energy increment
// mw= Energy and z dependence mass in well
// mb= Energy and z dependence mass in barrier
// i=0 For conduction band,i=1 for LH,i=2 for HH
// .....

int
main ()
{
    FILE *fp, *sfp;
    double vp, Ec[40], Eh[40], El[40], x[MAX_SAMPLES], wellw;
    double temp, templ, ML, Eg_InSb;
    double Egw, Egb, vs, a, b, EgHH, EgLH;
    double Egw_lh, vp_lh;
    double delb;
    double hhconf[MAX_SAMPLES], lhconf[MAX_SAMPLES];
    int h, i, j, k;
    int nsol, nsol_lh, nsol_hh;
    double a_old, b_old;
    double hhmod[MAX_SAMPLES], lhmod[MAX_SAMPLES];
    double lh_weight[MAX_SAMPLES], hh_weight[MAX_SAMPLES];
    double xst[MAX_SAMPLES], a2_prime;
    double hh_slope_l, hh_int_l, lh_slope_l, lh_int_l;

```

```

double hh_minus_bdep[MAX_SAMPLES];
double hhy[MAX_SAMPLES], lhy[MAX_SAMPLES];
double ohhy[MAX_SAMPLES], olhy[MAX_SAMPLES];
double hh_err[MAX_SAMPLES], lh_err[MAX_SAMPLES];
int bc, nsamp;
int stat_iterations, gap_feedback;
double lh_minus_hh[MAX_SAMPLES];
double a_sum, b_sum, Eg_sum;
double a_sum2, b_sum2, Eg_sum2;
double a_mean, b_mean, Eg_mean;
double a_sd, b_sd, Eg_sd;

srand48 (time (NULL));

fp = fopen (OUTFILE, "w");
sfp = fopen (STATFILE, "w");

printf ("Check well width and Eg(InSb)!!! \n");

// Caution: Well Width defined by wellww[h] and number of monolayers below
a = -7.7; //Hydrostatic deformation potential (absolute value)
b = -2.05; //Shear deformation potential (absolute value)
ML = 15; //Number of monolayers for well
Eg_InSb = 0.236; //Bulk energy gap for InSb

nsamp = read_data (INFILE, x, ohhy, olhy, hh_weight, lh_weight,
                  hh_err, lh_err, MAX_SAMPLES);

// Eg_InSb=ohhy[0]; //FRED

stat_iterations = 0;
gap_feedback = 0;
read_params (INFILE, &a, &b, &Eg_InSb, &ML, &stat_iterations,
            &gap_feedback);

fprintf (fp, "Number of Monolayers: %lf Initial Eg_well= %lf\n", ML,
        Eg_InSb);
fprintf (fp, "Read %d samples from file\n", nsamp);
printf ("Read %d samples from file\n", nsamp);
for (i = 0; i < nsamp; i++)
    x[i] *= 0.01; //Convert from percentage

if (stat_iterations <= 1)
    stat_iterations = 1;

a_sum = 0.0;
b_sum = 0.0;
Eg_sum = 0.0; // Initialize stat variables
a_sum2 = 0.0;
b_sum2 = 0.0;
Eg_sum2 = 0.0;

for (k = 0; k < stat_iterations; k++) { // The Stat Loop
    if (stat_iterations > 1) {
        for (i = 0; i < nsamp; i++) {
            hhy[i] = ohhy[i] + randgauss (hh_err[i]);
            lhy[i] = olhy[i] + randgauss (lh_err[i]);
        }
    }
    else {
        for (i = 0; i < nsamp; i++) {
            hhy[i] = ohhy[i];
            lhy[i] = olhy[i];
        }
    }
}

```

```

    }
}

for (bc = 0; bc < 1000; bc++) {      // Start bigloop

    for (h = 0; h < nsamp; h++) {      // Loop for stepping through
        // concentration values
        // Delta value for barrier
        delb = (delw * (1 - x[h]) + delAlSb * x[h]);
        a2_prime = a1 * (1.0 - x[h]) + a3 * x[h];

        if (x[h] == 0.0) {            //Skip Zero Concentration
            hhy[h] = Eg_InSb;
            lhy[h] = Eg_InSb;
            hhconf[h] = 0.0;
            lhconf[h] = 0.0;
            continue;
        }

        //          ww=15*(a1*a1*a1)/((a2*a2)*2);
        //Well width based on number of monolayers and
        //strain expansion of lattice constant in growth direction. Assumes constant
        //volume of InSb cell:  a_2=Vol/(((a_alloy)^2)/2)
        wellw = ML * (a1 * a1 * a1) / (2.0 * a2_prime * a2_prime);

        //          fprintf(fp,"a1= %le x= %le a= %lf b= %lf \n",a1,x,a,b);

        Egb = (Eg_InSb + 2.06143 * x[h]);
        Egw =
            (Eg_InSb +
             (a * (2.0 - 2.0 * 0.548) - b * (1.0 + 2.0 * .548)) * st);
        vs = (Egb - Egw) * band_offset;
        vp = vs + (Egw - Egb);
        Egw_lh =
            (Eg_InSb +
             (a * (2.0 - 2.0 * 0.548) + b * (1.0 + 2.0 * .548)) * st -
             (9.0 / (4.0 * delw)) * b * b * (1.0 + 2.0 * 0.548) *
             (1.0 + 2.0 * 0.548) * st * st);

        //          Egw_lh =
        //          Eg_InSb + a * (2.0 - 2.0 * 0.548) * st +
        //          (delw / 2) * (1 - (-b) * (1.0 + 2.0 * .548) * st / delw) -
        //          (delw / 2) * sqrt ((1 + 2 * (-b) * (1.0 +
        //          2.0 * .548) * st / delw) + 9 * ((-b) *
        //          (1.0 + 2.0 * .548) * st / delw) * ((-b) *
        //          (1.0 + 2.0 * .548) * st / delw));

        vp_lh = vs + (Egw_lh - Egb);

        fprintf (fp, "Concentration: %lf%%\n", x[h] * 100.0);

        fprintf (fp, "*****Conduction Band *****\n");
        nsol =
            e_solver (Egw * cf, Egb * cf, vs * cf, vp * cf, delb * cf,
                      wellw, 0.0, vs * cf, de * cf, 1, Ec);
        for (j = 0; j < nsol; j++)
            Ec[j] = 1000.0 * Ec[j] / cf;
        fprintf (fp, "Found 3d energies:\n", nsol);
        fprintf (fp, "Ec: %lf\n", Ec[0]);

        fprintf (fp, "*****LH Band *****\n");
        nsol_lh =
            e_solver (Egw_lh * cf, Egb * cf, vs * cf, vp_lh * cf,
                      delb * cf, wellw, -Egw_lh * cf,

```

```

        (-Egw_lh + vp_lh) * cf, -de * cf, 1, El);
for (j = 0; j < nsol_lh; j++)
    El[j] = 1000.0 * fabs (Egw_lh * cf + El[j]) / cf;
fprintf (fp, "Found %d energies:\n", nsol_lh);
fprintf (fp, "El: %lf\n", El[0]);
fprintf (fp, "*****HH Band *****\n");
nsol_hh =
    e_solver (Egw * cf, Egb * cf, vs * cf, vp * cf, delb * cf,
              wellw, -Egw * cf, (-Egw + vp) * cf, -de * cf, 2,
              Eh);
for (j = 0; j < nsol_hh; j++)
    Eh[j] = 1000.0 * fabs (Egw * cf + Eh[j]) / cf;
fprintf (fp, "Found %d energies:\n", nsol_hh);
fprintf (fp, "Eh: %lf\n", Eh[0]);

EqHH = Egw;
EqLH = Egw_lh;

fprintf (fp, "EqHH=%lf EqLH=%lf \n", EqHH, EqLH);
fprintf (fp, " \n \n ");
fprintf (fp, "Initial Eg for well = %le eV \n", Eg_inSb);
fprintf (fp, "Well width=%le \n", wellw / (1.0e-8));
fprintf (fp, "a1= %le x= %le a= %lf b= %lf \n \n", a1, x[h],
        a, b);
fprintf (fp, "HH1-CB1= %le \n ",
        (Ec[0] + Eh[0] + EqHH * 1000));
fprintf (fp, "LH1-CB1= %le \n \n ",
        (Ec[0] + El[0] + EqLH * 1000));

if (nsol * nsol_hh != 0) {
    fprintf (fp, "HHconf= %le \n ", (Ec[0] + Eh[0]));
    hhconf[h] = (Ec[0] + Eh[0]) / 1000;
}
else {
    fprintf (fp,
              "WARNING: No solution for the heavy hole
confinement!\n");
    fprintf (fp, "Setting hhconf=0!\n");
    hhconf[h] = 0.0;
}

if (nsol * nsol_lh != 0) {
    fprintf (fp, "LHconf= %le \n \n \n", (Ec[0] + El[0]));
    lhconf[h] = (Ec[0] + El[0]) / 1000;
}
else {
    fprintf (fp,
              "WARNING: No solution for the light hole
confinement!\n");
    fprintf (fp, "Setting lhconf=0!\n");
    lhconf[h] = 0.0;
}

} //Close loop for stepping through concentration
values

// Print observed transition energies: hhl
fprintf (fp, "\n\nObserved energies:\n");
for (i = 0; i < nsamp; i++) {
    fprintf (fp, "%14.8lf ", x[i]);
    if (hh_weight[i] == 0.0)
        fprintf (fp, "%14s ", "");
    else

```

```

        fprintf (fp, "%14.8lf ", hhy[i]);
        if (lh_weight[i] == 0.0)
            fprintf (fp, "%14s ", "");
        else
            fprintf (fp, "%14.8lf ", lhy[i]);
        fprintf (fp, "\n");
    }
    //End print observed energies loop

//Print the modified energies: Observed minus confinement
//Caution: Earlier confinement values start from x=0.053 and we need x=0 here
    for (i = 0; i < nsamp; i++) {
        hhmod[i] = hhy[i] - hhconf[i];
        lhmod[i] = lhy[i] - lhconf[i];
    }

    fprintf (fp, "\n\n\nModified energies!!!\n");
    for (i = 0; i < nsamp; i++) {
        fprintf (fp, "%14.8lf ", x[i]);
        if (hh_weight[i] == 0.0)
            fprintf (fp, "%14s ", "");
        else
            fprintf (fp, "%14.8lf ", hhmod[i]);
        if (lh_weight[i] == 0.0)
            fprintf (fp, "%14s ", "");
        else
            fprintf (fp, "%14.8lf ", lhmod[i]);
        fprintf (fp, "\n");
    }
    //End print modified energies

// Calculate x*st for linear fits
    for (i = 0; i < nsamp; i++) {
        a2_prime = a1 * (1.0 - x[i]) + a3 * x[i];
        xst[i] = (a2_prime - a1) / a1;
        fprintf (fp, "STS: %1f %1f\n", x[i], xst[i]);
    }

    a_old = a;
    b_old = b;

    for (i = 0; i < nsamp; i++)
        lh_minus_hh[i] = lhmod[i] - hhmod[i];

    nonlin_fit (xst, lh_minus_hh, lh_weight, nsamp, sb);
    fprintf (fp, "Non lin b=%1f\n", b);

    for (i = 0; i < nsamp; i++)
        hh_minus_bdep[i] =
            hhmod[i] + b * (1.0 + 2.0 * 0.548) * xst[i];

    linear_least_squares (xst, hh_minus_bdep, hh_weight, nsamp,
        &hh_slope_1, &hh_int_1);

    a = (hh_slope_1) / (2.0 + 2.0 * .548);
    fprintf (fp, "Intercept=%1f \n", hh_int_1);
    if (gap_feedback)
        Eg_InSb = hh_int_1;

    fprintf (fp, "New values: \n a=%1f   b=%1f   \n", a, b);

    if ((fabs ((a_old - a) / a) < 0.0001)
        && (fabs ((b_old - b) / b) < 0.0001)) {
        fprintf (fp, "Number of iterations was: %d\n", (bc + 1));
        break;
    }

```

```

    }
    // End big loop

    fprintf (sfp, "%1f %1f %1f\n", a, b, Eg_InSb);

    a_sum += a;          // Calculate statistics
    b_sum += b;
    Eg_sum += Eg_InSb;
    a_sum2 += a * a;
    b_sum2 += b * b;
    Eg_sum2 += Eg_InSb * Eg_InSb;

} // End Stat Loop

a_mean = a_sum / stat_iterations;
b_mean = b_sum / stat_iterations;
Eg_mean = Eg_sum / stat_iterations;
if (stat_iterations > 1) {
    a_sd = (a_sum2 - a_mean * a_sum) / (stat_iterations - 1);
    if (a_sd < 0.0)
        a_sd = 0.0;
    else
        a_sd = sqrt (a_sd);
    b_sd = (b_sum2 - b_mean * b_sum) / (stat_iterations - 1);
    if (b_sd < 0.0)
        b_sd = 0.0;
    else
        b_sd = sqrt (b_sd);
    Eg_sd = (Eg_sum2 - Eg_mean * Eg_sum) / (stat_iterations - 1);
    if (Eg_sd < 0.0)
        Eg_sd = 0.0;
    else
        Eg_sd = sqrt (Eg_sd);
}
else {
    b_sd = 0.0;
    a_sd = 0.0;
    Eg_sd = 0.0;
}

fprintf (sfp, "\nFinal statistics\n-----\n");
fprintf (sfp, "a   mean:%10lf   std dev: %10lf\n", a_mean, a_sd);
fprintf (sfp, "b   mean:%10lf   std dev: %10lf\n", b_mean, b_sd);
fprintf (sfp, "Eg  mean:%10lf   std dev: %10lf\n", Eg_mean, Eg_sd);

fclose (fp);
fclose (sfp);

return 0;

} // end main

```

D.2. Drand48.cpp

This software originated from the Free Software Foundation under the GNU libC library.

```
/*      @(#)drand48.c                                2.2
 */

/*LINTLIBRARY*/

/*
 *
 *      drand48, etc. pseudo-random number generator
 *
 *      This implementation assumes unsigned short integers of at least
 *
 *      16 bits, long integers of at least 32 bits, and ignores
 *
 *      overflows on adding or multiplying two unsigned integers.
 *
 *      Two's-complement representation is assumed in a few places.
 *
 *      Some extra masking is done if unsigneds are exactly 16 bits
 *
 *      or longs are exactly 32 bits, but so what?
 *
 *      An assembly-language implementation would run significantly faster.
 *
 */

#ifndef HAVEFP
#define HAVEFP 1
#endif

#define N      16

#define MASK    ((unsigned)(1 << (N - 1)) + (1 << (N - 1)) - 1)

#define LOW(x)  ((unsigned)(x) & MASK)

#define HIGH(x)  LOW((x) >> N)

#define MUL(x, y, z) { long l = (long)(x) * (long)(y); \
                        (z)[0] = LOW(l); (z)[1] = HIGH(l); }

#define CARRY(x, y) ((long)(x) + (long)(y) > MASK)

#define ADDEQU(x, y, z) \
    CARRY(x, (y)), x = LOW(x + (y)))
```

(z =


```

#define X0      0x330E

#define X1      0xABCD

#define X2      0x1234

#define A0      0xE66D

#define A1      0xDEEC

#define A2      0x5

#define C      0xB

#define SET3(x, x0, x1, x2)          ((x)[0] =
(x0), (x)[1] = (x1), (x)[2] = (x2))

#define SETLOW(x, y, n) SET3(x, LOW((y)[n]), LOW((y)[(n)+1]), LOW((y)[(n)+2]))

#define SEED(x0, x1, x2) (SET3(x, x0, x1, x2), SET3(a, A0, A1, A2), c = C)

#define REST(v)      for (i = 0; i < 3; i++) { xsubi[i] = x[i]; x[i] = temp[i]; } \

                        return (v);

#define NEST(TYPE, f, F)              TYPE f
register unsigned short *xsubi) { \

    register int i; register TYPE v; unsigned temp[3]; \

    for (i = 0; i < 3; i++) { temp[i] = x[i]; x[i] = LOW(xsubi[i]); } \

    v = F(); REST(v); }

#define HI_BIT      (1L << (2 * N - 1))

static unsigned x[3] = { X0, X1, X2 }, a[3] = { A0, A1, A2 }, c = C;

static unsigned short lastx[3];

static void nextt();

#if HAVEFP

double

drand48()

{

#if pdp11

```

```

static double two16m; /* old pdp11 cc can't compile an expression */

two16m = 1.0 / (1L << N); /* in "double" initializer! */

#else

static double two16m = 1.0 / (1L << N);

#endif

nextt();

return (two16m * (two16m * (two16m * x[0] + x[1]) + x[2]));
}

```

NEST(double, erand48, drand48);

#else

long

irand48(m)

/* Treat x[i] as a 48-bit fraction, and multiply it by the 16-bit

* multiplier m. Return integer part as result.

*/

register unsigned short m;

{

unsigned r[4], p[2], carry0 = 0;

nextt();

MUL(m, x[0], &r[0]);

MUL(m, x[2], &r[2]);

MUL(m, x[1], p);

if (CARRY(r[1], p[0]))

```

        ADDEQU(r[2], l, carry0);

    return (r[3] + carry0 + CARRY(r[2], p[1]));
}

long
krand48(xsubi, m)

/* same as irand48, except user provides storage in xsubi[] */
register unsigned short *xsubi;
unsigned short m;
{
    register int i;
    register long iv;
    unsigned temp[3];

    for (i = 0; i < 3; i++) {
        temp[i] = x[i];
        x[i] = xsubi[i];
    }

    iv = irand48(m);
    REST(iv);
}

#endif

long
lrnd48()
{
    nextl();

    return (((long)x[2] << (N - 1)) + (x[1] >> 1));
}

```

```

}

long
mrand48()
{
    register long l;

    next();

    /* sign-extend in case length of a long > 32 bits

        (as on Honeywell) */

    return ((l = ((long)x[2] << N) + x[1]) & HI_BIT ? l | -HI_BIT : l);
}

static void
next()
{
    unsigned p[2], q[2], r[2], carry0, carry1;

    MUL(a[0], x[0], p);
    ADDEQU(p[0], c, carry0);
    ADDEQU(p[1], carry0, carry1);
    MUL(a[0], x[1], q);
    ADDEQU(p[1], q[0], carry0);
    MUL(a[1], x[0], r);
    x[2] = LOW(carry0 + carry1 + CARRY(p[1], r[0]) + q[1] + r[1] +
        a[0] * x[2] + a[1] * x[1] + a[2] * x[0]);
    x[1] = LOW(p[1] + r[0]);
    x[0] = LOW(p[0]);
}

```

```

}

void
srand48(long seedval)
{
    SEED(X0, LOW(seedval), HIGH(seedval));
}

unsigned short *
seed48(unsigned short seed16v[3])

{
    SETLOW(lastx, x, 0);

    SEED(LOW(seed16v[0]), LOW(seed16v[1]), LOW(seed16v[2]));

    return (lastx);
}

void
lcong48(unsigned short param[7])
{
    SETLOW(x, param, 0);

    SETLOW(a, param, 3);

    c = LOW(param[6]);
}

NEST(long, mrand48, lrand48);

NEST(long, jrand48, mrand48);

```

```
#ifndef DRIVER
```

```
/*
```

```
    This should print the sequences of integers in Tables 2
```

```
    and 1 of the TM:
```

```
    1623, 3442, 1447, 1829, 1305, ...
```

```
    657EB7255101, D72A0C966378, 5A743C062A23, ...
```

```
*/
```

```
#include <stdio.h>
```

```
main()
```

```
{
```

```
    int i;
```

```
    for (i = 0; i < 80; i++) {
```

```
        printf("%4d ", (int)(4096 * drand48()));
```

```
        printf("%.4X%.4X%.4X\n", x[2], x[1], x[0]);
```

```
    }
```

```
}
```

```
#endif
```

D.3. Samples.in

```
a  = -7.7
b  = -2.05
Eg = 0.239
ML = 16
StatIterations=1
GapFeedback=0
data
  0.0  0.239  0.239  0.002  0.002
  4.92 0.3195  NA    0.003  NA
 11.1  0.3779  0.4303 0.002  0.0025
 20.7  0.4336  0.5393 0.002  0.007
 32.2  0.4782  0.635  0.003  0.0045
```

Appendix E. Program To Calculate Conduction Subband Dispersion Curves

E.1. Qwkt_d.bas

```

REM FRED   I've modified some, finished in this 3rd version
REM Program calculates E(l,kt, for InSb/InAlSb quantum wells

DIM KT(100)
DIM E(10, 100)
DIM ECRIT(100)

DECLARE SUB SUB1 (E, DE, EO, EI, V, MO, M1, HB, CF, KT, B, K, Q, B2, d)
DECLARE SUB SUB2 (E, DE, EO, EI, V, MO, M1, HB, CF, KT, B, K, Q, B2, d)
DECLARE SUB SUB3 (E(), IMAX, KT(), JMAX, KTINC, HB, M2, CF)

REM FRED The next line added by Fred
PRINT "Input a file name for data "
INPUT file1$
OPEN "O", #1, file1$
PRINT "Filename for the data: "; file1$

PRINT "QW thickness in cm="
INPUT d
PRINT "Al conc.="
INPUT X
PRINT "Band offset ratio="
INPUT C
PRINT "Well strained enter 0; barrier strained enter 1"
INPUT FL
PRINT "d="; d
PRINT "Al conc.="; X
PRINT "Band offset ratio="; C
IF FL = 0 THEN PRINT "Well strained"
IF FL = 1 THEN PRINT "Barrier strained"

REM Lattice parameters and strain
A1 = 6.479E-08           'InSb
A3 = 6.136E-08           'AlSb
A2 = A1 * (1 - X) + A3 * X   'InSbSb

REM Unstrained 4K energy gaps
EO = .236                'InSb
EI = EO + 2! * X          'InAlSb

REM Strained 4K energy gaps
IF FL = 0 THEN
    LET ST = (A2 - A1) / A1
    LET EO = EO + (-7.7 * (2 - 2 * .546) + 2.05 * (1 + 2 * .546)) * ST
ELSE
    LET CR = .546 - .068 * X

```



```

      LET A = -7.7 + 1.8 * X
      LET B = -2.05 + .7 * X
      LET ST = (A1 - A2) / A2
      LET E1 = E1 + (A * (2 - 2 * CR) + B * (1 + 2 * CR)) * ST
END IF

REM Masses and g-factors

M0 = 1 / (-2! + (23.5 / 3) * (2 / E0 + 1 / (E0 + .8)))
M1 = 1 / (-2! + (23.5 / 3) * (2 / E1 + 1 / (E1 + .8)))
G0 = -2! * (1 / M0 + 2!) * (.8 / (3 * E0 + 1.6))
G1 = -2! * (1 / M1 + 2!) * (.8 / (3 * E1 + 1.6))

REM Band offset from offset ratio

V = (0 - .5) * (E1 - E0)
PRINT "Egap(well)", "Egap(barrier)", "band offset"
PRINT E0, E1, V
PRINT "well mass", "barrier mass"
PRINT M0, M1
PRINT "well g-factor", "barrier g-factor"
PRINT G0, G1

REM Physical constants

HB = 1.054E-27
M2 = 9.11E-28
CF = 1.602E-12

REM KT increment and number of KT values

PRINT "KT interval="
INPUT KTINC
PRINT "Number of KT values less one="
INPUT JMAX

PRINT "KT interval="; KTINC
PRINT "Number of KT values less one="; JMAX

REM Convert to cgs units

E0 = E0 * CF
E1 = E1 * CF
DE = .001 * CF
V = V * CF
M0 = M0 * M2
M1 = M1 * M2

REM KT loop

FOR J = 0 TO JMAX
  LET KT(J) = J * KTINC
  KT = KT(J)
  IMAX = 0

  REM Energy loop

  FOR N = 1 TO 2000
    LET E = .001 * N * CF + E0 / 2
    LET FLAG = 0
    CALL SUB1(E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)
    IF B2 <= 0 THEN

```

```

        LET FLAG = 1
        LET ZZ = E1 * KT * KT / (2 * M1 / HB / HB) + E1 * E1 / 4
        LET E = V + SQR(ZZ)
REM FRED The line below prints k,E (which is ECRIT) for the 3rd Subband
        ECRIT(J) = E / CF - E0 / CF / 2
REM FRED        WRITE #3, KT(J), E / CF - E0 / CF / 2
        CALL SUB1(E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)
        END IF
        LET W = Q
        IF (Q <= 0 AND G >= 0 AND K <> 0) THEN
REM FRED In SUB2, k,E are printed for the 1st Subband
                CALL SUB2(E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)
                E(IMAX, J) = E / CF - E0 / CF / 2
                IMAX = IMAX + 1
                LET G = W
        ELSEIF (Q <= 0 AND G < 0) THEN
                LET G = W
        ELSEIF Q > 0 THEN
                LET G = W
        END IF
        IF FLAG = 1 THEN EXIT FOR
    NEXT N
REM FRED    FOR I = 0 TO IMAX - 1

REM FRED    NEXT I

REM FRED These next lines print k,E for the 1st and 2nd Subband, respectively
REM FRED WRITE #1, KT(J), E(0, J)
REM FRED WRITE #2, KT(J), E(1, J)
WRITE #1, KT(J), E(0, J), E(1, J), E(2, J), E(3, J), E(4, J), E(5, J), E(6, J),
E(7, J), E(8, J), E(9, J), ECRIT(J)
NEXT J
CALL SUB3(E(), IMAX, KT(), JMAX, KTINC, HB, M2, CF)
END

SUB SUB1 (E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)

REM Well dispersion

K2 = (2 * M0 / HB) * (E * E - E0 * E0 / 4) / HB / E0 - KT * KT

REM Barrier dispersion

B2 = (2 * M1 / HB) * (E1 * E1 / 4 - (E - V) ^ 2) / HB / E1 + KT * KT

IF B2 < 0 THEN B2 = 0
B = SQR(B2)                                'kappa
IF K2 < 0 THEN K2 = 0
K = SQR(K2)                                'k
R = (E - V + E1 / 2) / (E + E0 / 2)

REM Matching boundary condition

IF K = 0 THEN
    LET Q = B ^ 2 - (KT * (R - 1) / 2) ^ 2
ELSE
    LET Q = (B + K * R / TAN(K * d / 2)) * (B - K * R * TAN(K * d / 2))
    LET Q = Q - (KT * (R - 1) / 2) ^ 2
END IF
END SUB

SUB SUB2 (E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)

REM Root finder subroutine

```

```

FOR m = 1 TO 10
    E = E + SGN(Q) * DE / (2 ^ m)
    CALL SUB1(E, DE, E0, E1, V, M0, M1, HB, CF, KT, B, K, Q, B2, d)
NEXT m

REM FRED The line below prints the k,E values for the 1st subband
REM FREDPRINT K, B
END SUB

SUB SUB3 (E(), IMAX, KT(), JMAX, KTINC, HB, M2, CF)
FOR I = 0 TO IMAX - 1
    NS = 0
    FOR J = 0 TO JMAX - 1
        REM Motional binding possibility
        IF E(I, J) > 0 THEN
            IF FLG = 1 THEN LET KC = KT(J)
            LET DEDK = (E(I, J + 1) - E(I, J)) / KTINC
            LET MSTAR = (HB / M2) * (HB / CF) * (KT(J) + KTINC / 2) / DEDK
            LET NS = NS + (KT(J) + KTINC / 2) * (E(I, J + 1) - E(I, J)) / DEDK /
3.14159
            LET NSR = (KT(J) + KTINC / 2) ^ 2 / 2 / 3.14159 - KC * KC / 2 / 3.14159
REM FRED      PRINT KT(J) + KTINC / 2, MSTAR, NS, NSR
        ELSE
            LET FLG = 1
        END IF
    NEXT J
NEXT I
END SUB

```