AN ABSTRACT OF THE THESIS OF


Abstract approved: ____________________________
John R. Arthur

This thesis reports on growth by molecular beam epitaxy (MBE) and characterization of III-V compound semiconductor materials for use in modulation doped field effect transistor (MODFET) structures and related devices. The first section of this work studies the effect of substrate orientation on carbon doping behavior in MBE grown GaAs. A series of carbon doped samples were grown on (100), (111A) and (111B) oriented substrates using volatile CBr₄ as the dopant source. All samples were found to be p-type and have mobilities comparable to beryllium doped samples of similar doping concentration.

The second part of this work investigates growth of high quality InGaAs by using reflection high energy electron diffraction (RHEED) to study growing InGaAs layers and by characterizing single quantum wells of InGaAs by photoluminescence. Effects of growth temperature, arsenic overpressure, growth stops and the use of AlₓGa₁₋ₓAs are
investigated. Results indicate that InGaAs quantum well quality can be improved by growth at substrate temperatures near 570°C and by including several monolayers of GaAs between the InGaAs channel layer and AlGaAs barrier layer in strained layer InGaAs MODFET structures.

The third section of this work studies a novel MODFET structure with a channel region made of GaAs grown at low substrate temperatures of ~250°C-350°C (LT-GaAs). Herein, the first study of a two dimensional electron gas (2DEG) in LT-GaAs is presented. Additionally, experimental mobility measurements at 77K (made for the first time in LT-GaAs) are found to be in good agreement with mobilities calculated using a computer simulation for MODFET structures using a first order model for the various scattering mechanisms including scattering from arsenic clusters present in annealed LT-GaAs layers.

A new photoluminescence line at 1.65eV is observed in all the LT-GaAs MODFET structures studied. This peak is believed to be caused by a spatially indirect transition from a 2DEG at the heterojunction interface to holes in the AsGaAs. The large light sensitivity exhibited by the LT-GaAs MODFET structure was exploited to fabricate photodetectors from this material. These devices were found to have an impressive responsivity of 65 A/W at 0.87μm photoexcitation and 6.5 A/W at 1.0μm.

by

Donald W. Schulte

A THESIS

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I understand that my thesis will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my thesis to any reader upon request.
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I would like to extend my thanks to a number of people who have helped me attain this goal. Special thanks to my co-advisors John Arthur and Stephen Goodnick who encouraged me to pursue my Ph.D. and who have provided me with valued guidance, insight and support over the past six years. Equally notable is my co-worker Leon Ungier, with whom I have spent countless hours in the lab working on these experiments and taking care of the necessary maintenance and repair of the equipment used in this work. In addition to his assistance in the lab, Leon has also been instrumental in the design of many of the experiments presented herein. Particularly notable were his observations of the RHEED phenomena which led to the experiments discussed in the second section of work. Although I have only had the opportunity to work with Dr. S. Subramanian for the past two years, the value of his contributions to this work are unquestionable. Close collaboration with Dr. Subramanian has made possible most of the work on LT-GaAs presented in section three of this thesis, from which several publications have resulted. Finally I would like to my mother and family who have supported me throughout this long journey.

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1. Introduction

Semiconductor technology has advanced extremely rapidly during its brief history. As a result of this rapid growth, the complexity of semiconductor devices and the constraints placed upon them have increased at a dramatic rate. Current semiconductor technologies are already approaching limits in size and complexity that were once thought to be physically impossible. As these technologies are further developed, there will be a continuing need to increase device density while maintaining or improving performance. In order to achieve these advances, novel devices, materials and fabrication techniques will have to be developed.

One important area in semiconductor technology development is that of epitaxial crystal growth. Epitaxial growth is the growth of crystalline semiconductor material upon a crystal substrate and can fall into two distinct classes. Homoepitaxy, or the growth of a semiconductor material upon a substrate of the same material defines one class of epitaxial growth. The growth of crystalline silicon upon a silicon substrate would be an example of homoepitaxial growth. Heteroepitaxy, or the crystalline growth of one semiconductor material upon a substrate of a different material defines the other class of epitaxy. The growth of III-V compound semiconductors such as InGaAs or AlGaAs upon GaAs substrate material is an example of heteroepitaxial growth and will be the primary focus of discussion in this thesis.

In epitaxial growth, the interface between two dissimilar semiconductor materials is referred to as a heterointerface. Since different semiconductor materials generally have
characteristics which dramatically differ, it is possible to have very abrupt changes in material properties at a heterointerface. Using these abrupt changes in material composition novel semiconductor structures can be created to allow the fabrication of new devices and the study of specific material properties.

The use of epitaxial growth allows the abrupt change of many different material properties. One of the most important properties that can be controlled is the conductivity of a material, which is determined by the type and concentration of impurities present in the crystal. In many types of epitaxial growth and especially in Molecular Beam Epitaxy (MBE), both the concentration and type of impurities can be precisely controlled, allowing the conductivity of a sample to be tailored to meet specific design needs. For example, by using MBE, layers of a material heavily doped with an n-type impurity can be easily grown upon either lightly doped n-type material or material doped with a p-type impurity.

In the growth of III-V compound semiconductors by MBE, silicon is commonly used as an n-type impurity and beryllium is the most common p-type impurity. However, beryllium exhibits significant diffusion [1] and surface segregation [2] in GaAs, and both of these effects can be extremely detrimental to the performance of many devices. It would be desirable to find an alternative p-type dopant which does not have these problems. Recently, carbon has been investigated as a possible alternative to beryllium for p-type doping in GaAs. Research on carbon doping in the III-V semiconductors has demonstrated that in addition to having a high level of electrical activity, carbon also has a much lower diffusion coefficient than other p-type impurities such as beryllium and zinc. [3,4,5] Consequently, carbon appears to be a promising candidate for p-type doping in
GaAs, but many more properties of carbon doped GaAs need to be studied to fully understand the nature of carbon impurities in GaAs. Some studies of carbon doping are reported in Chapter 3.

Another important property that can be altered abruptly in heteroepitaxy is the bandgap of a semiconductor. Since differing semiconductor materials normally have different bandgaps, a potential discontinuity must appear in the conduction and valence bands at the heterointerface in order to accommodate the bandgap difference between the two materials. By growing semiconductor materials with one or more heterointerfaces, the bandgap discontinuities which result at each heterointerface can be used to create new semiconductor structures with novel band profiles and new properties. The second part of this work addresses the growth of high quality InGaAs, a technologically important III-V semiconductor.

Because of its narrower bandgap and higher carrier mobilities, InGaAs is an important material used in many III-V semiconductor devices. Since the bandgap of InGaAs is much smaller than that of GaAs, the growth of thin layers of InGaAs within GaAs creates an important class of structures which exhibit quantum confinement effects. In the area of fiber optics communications, there is a need for laser diodes that operate at a wavelength of 1.3\textmu m or 1.5\textmu m to take advantage of the minimum loss of silica fibers. In order to realize this operating wavelength, laser diodes frequently use a quantum well of a narrow bandgap semiconductor such as InGaAs for the active region. The reasonably large carrier mobility of InGaAs has also made it important for use in several types of high
speed field effect devices such as the pseudomorphic heterostructure field effect transistor (pHFET).

The performance of all of these devices depends greatly upon the quality of the InGaAs layer that can be grown. The growth of InGaAs upon GaAs is complicated by the fact that InAs and GaAs have a lattice mismatch of approximately 7%. However, it has been shown by Matthews and Blakeslee [6,7,8] that the epitaxial growth of highly mismatched structures is possible if the thickness of the epilayer is below a critical thickness which depends on the mismatch. If an $\text{In}_y\text{Ga}_{1-y}\text{As}$ layer is grown thin enough, the lattice mismatch will be absorbed as strain in the $\text{In}_y\text{Ga}_{1-y}\text{As}$, causing the in-plane lattice constant of $\text{In}_y\text{Ga}_{1-y}\text{As}$ to conform to the lattice constant of the GaAs substrate, yielding a pseudomorphic $\text{In}_y\text{Ga}_{1-y}\text{As}$ layer. Another complication in the growth of high quality InGaAs is the extreme sensitivity of InGaAs to the growth conditions. InGaAs is typically grown at lower temperatures than GaAs due to the significantly increased segregation and reevaporation of indium from the growth surface at temperatures normally used for GaAs growth. Due to the complications involved in the growth of InGaAs, it is important to understand and optimize the growth conditions for the growth of high quality InGaAs layers.

In order to further the understanding of some of the problems associated with growth in the complicated InGaAs material system, this portion of this work addresses the growth of high quality InGaAs layers on GaAs. The growth of InGaAs is investigated by reflection high energy electron diffraction (RHEED) studies of the growing InGaAs layers and by characterization of single quantum wells of InGaAs by photoluminescence are all
investigated. Since many technologically important device structures use Al$_x$Ga$_{1-x}$As overlayers directly on top of InGaAs quantum wells, rather than GaAs overlayers, the effects of using both GaAs and Al$_x$Ga$_{1-x}$As overlayers are studied in conjunction with the effects of growth temperature, arsenic overpressure, and stop growths.

Although the growth of high quality GaAs layers is experimentally simpler than the growth of high quality InGaAs layers, the growth temperature used still can have dramatic effects upon the properties of GaAs. The third part of this work studies the growth of GaAs at low temperatures of 200 - 350°C (LT-GaAs) and the properties of this material, which recently has become important for use in high speed optical detectors and transistors. It has been shown that LT-GaAs as grown is non-stoichiometric with an excess arsenic concentration on the order of 1% [9] and is moderately conducting. The excess arsenic precipitates in the form of small arsenic clusters when the sample is annealed at a temperature of ~600°C and the material then becomes highly resistive [10]. Due to the extremely large resistivity of annealed LT-GaAs, it has been found to be an excellent buffer layer for devices such as metal-semiconductor field effect transistors (MESFETs) and modulation-doped field effect transistors (MODFETs). [11,12] LT-GaAs also has an extremely short (~1ps) excess carrier lifetime [13,14], and has shown promise for use in high speed photodetectors.

Although the large resistivity of LT-GaAs makes it ideal for use as a buffer layer, it also presents extreme difficulty in characterizing the transport properties of this material by conventional experimental techniques such as Hall effect measurements. Due to this difficulty, there has been only limited progress in understanding the transport properties of
LT-GaAs. In the third part of this work a novel MODFET structure, in which the channel region is made of LT-GaAs, is used to investigate the transport properties of LT-GaAs. This structure was found to have a large light sensitivity which allowed the reproducible measurement of Hall mobility under strong illumination. Using this new structure, it has been possible to measure the mobility of a two dimensional electron gas (2DEG) in LT-GaAs at both 300K and 77K. A simple scattering model for the arsenic clusters has been incorporated into a first order simulation of the mobility in this structure, and these calculations have shown good agreement with experimental results.

The large light sensitivity of the LT-GaAs MODFET suggested that the structure might have a potential use in photodetector applications requiring large sensitivity. To study the light sensitivity of the LT-GaAs MODFET structure more carefully, simple interdigitated metal-semiconductor-metal (MSM) photodetectors were fabricated on the material. These photodetectors were shown to be very sensitive with a 65A/W peak sensitivity in the GaAs bandgap energy range and a 6A/W peak sensitivity in the sub-bandgap energy region. The detectors showed a significant sub-bandgap response out to ~1.3 μm. The LT-GaAs MODFET was further characterized by using photoluminescence (PL) measurements. Previous experiments have shown little or no photoluminescence from LT-GaAs material; however, PL measurements on the LT-GaAs MODFET structure revealed a new peak at an energy between the bandgap of the GaAs channel region and that of the Al$_{0.2}$Ga$_{0.8}$As barrier layers. These results and the possible origins of this new PL peak will be discussed in section 3 of this thesis.
The three parts of this work attempt to examine fundamental aspects of material growth and their effect upon the optical and electrical properties of the material. The materials studied in this work all have significant importance for use in MODFET and opto-electronic device structures. The work on carbon doping studies the use of a relatively new p-type doping impurity which might be used as an alternative to beryllium for the growth of p-channel MODFETS or optical devices such as laser diodes. The properties of InGaAs such as a small direct bandgap, high carrier mobility, and the strain present in InGaAs layers grown on GaAs, make this an important material for use in MODFET and opto-electronic devices. The growth of GaAs at low temperatures investigates a new class of materials which have extremely low conductivity and extremely short carrier lifetimes, and thus are important for use as high resistivity buffer layers and in high speed photodetectors. An example of a device in which all three areas of this work might be combined is a p-channel MODFET using carbon doped AlGaAs barrier layers, an InGaAs channel to improve carrier mobility and quantum confinement, and a buffer layer of LT-GaAs to help reduce sidegating effects. As a whole, the results presented in this work are intended to provide a better overall understanding of several important areas of III-V semiconductor material growth, which will allow the creation of new and improved materials and devices.
2. Experimental Details.

2.1 MBE System Description.

The samples used for all parts of this work were grown by solid source Molecular Beam Epitaxy (MBE) in a Perkin Elmer Phi-425B MBE system. This system consists of three main high vacuum chambers. Sample introduction into the system is accomplished through a small volume introduction chamber isolated from the main system by an interlock valve. This allows the introduction chamber to be raised to atmospheric pressure and subsequent to sample exchange, be re-evacuated to a pressure of approximately $10^{-6}$ Torr without breaking the ultra high vacuum (UHV) environment of the main system chambers. Once the introduction chamber has been evacuated to a sufficiently low pressure, sample exchange mechanisms allow samples to be transferred from the introduction chamber into the main UHV chambers with minor impact on the main system vacuum.

The other two main system chambers, an analysis chamber and the growth chamber, are both maintained at a nominal pressure of $\sim 10^{-10}$ torr using ion pumps. The analysis chamber is connected between the introduction chamber and the growth chamber and contains an in-situ Auger Electron Spectrometer for surface analysis of samples, a heating stage where samples can be outgassed after introduction or heated during Auger analysis if necessary, and a space where several samples can be stored in the UHV environment.
The growth chamber in this system contains eight growth material sources and several in-situ analysis tools. Most of the source material is provided by solid sublimation sources including 2 gallium ovens, one indium oven and one aluminum oven for material growth, and silicon and beryllium ovens for n and p type doping respectively. The system at Oregon State University has also been fitted with a gaseous carbon-tetrabromide source controlled with a precision UHV compatible leak valve. This source provides an efficient and reliable method of growing p-type carbon doped III-V materials for novel research and devices. The arsenic flux in this system is produced by the sublimation of solid arsenic which yields $\text{As}_4$, which is then subsequently passed through a cracker to produce $\text{As}_2$ for growth.

Three in-situ analysis tools are present in the growth chamber of this system. A Quadrupole Mass Spectrometer (or Quadrupole Mass Analyzer (QMA)) is included in the growth chamber and can be used either to monitor the cleanliness of the system vacuum prior to sample growth (or post growth) or to analyze the composition of the fluxes from the sources during sample growth. Sample substrate temperature is monitored using an optical pyrometer which is mounted in line of sight with the growth stage. Finally, sample crystallography can be examined before, during and after growth by using Reflection High Energy Electron Diffraction as described in detail in the next section.
2.2 RHEED Oscillation Measurements.

The RHEED (Reflection High Energy Electron Diffraction) system consists of an electron gun incident at a glancing angle to the sample surface, where the beam is diffracted by the sample surface and focused onto a phosphor screen opposite the electron gun. Since a diffraction pattern is a representation of general crystal order in reciprocal space, and is an average of many unit cells, an electron beam incident at a glancing angle to an ordered crystal surface will produce a diffraction pattern of elongated lines which correspond to the lattice position of surface atoms. The distance between the lines and relative shape of a RHEED pattern will be inversely proportional to the actual surface crystal structure of the sample being analyzed. Surfaces with little or no crystal structure will not produce a pattern with elongated streaks due to the random orientation of the surface atoms. Therefore, the quality and shape of a RHEED pattern give a direct indication of the crystal quality of a surface, and can be used to ensure that good quality crystalline material is being grown.

There will also be some amount of specular reflection of the electron beam from a surface which will appear as a small bright spot in the center of the RHEED pattern. It has been shown that during the growth of crystal material, the intensity of this specularly reflected RHEED spot will oscillate, and that each oscillation in the RHEED pattern intensity represents the growth of a single monolayer of atoms on the crystal surface. [15] Thus, by monitoring the intensity of the RHEED oscillations as a function of time, the crystal growth rate can be calculated. In our system, this is accomplished by using an
optical fiber, which can be aligned to the specularly reflected RHEED spot, to couple the intensity of the RHEED pattern to a photomultiplier tube. The output of the photomultiplier tube is then monitored using a digital storage oscilloscope. From the trace of the digital storage oscilloscope, the number of intensity oscillations occurring in a given period of time can be counted and a growth rate in monolayers per second can be calculated.

This ability of RHEED measurements to determine surface crystallinity and measure growth rate, allow RHEED measurements to characterize two fundamental growth parameters. First, RHEED measurements allow the accurate design of complicated structures since both the material composition and the growth time to obtain a desired layer thickness can be calculated using this measurement. By adjusting the oven temperature of a particular source oven (thereby controlling the source material flux) and measuring the growth rate using RHEED oscillations, a desired growth rate for that oven can be obtained. For example the oven temperature of a Ga oven could be set such that a growth rate of 0.8 monolayers/sec. is obtained and an Al oven could likewise be set to produce a growth rate of 0.2 monolayers/sec. Then by growing with both of these ovens simultaneously, Al$_{0.2}$Ga$_{0.8}$As could be grown at a nominal growth rate of 1.0 monolayer/sec.

Another important use of RHEED measurements is in determining the substrate temperature of the sample. GaAs prepared for sample growth will have a thin native oxide layer on its surface. Since the oxide layer is amorphous, the RHEED pattern from a newly introduced GaAs sample will be generally featureless. As the sample is heated up to
growth temperatures, the oxide will eventually desorb from the GaAs surface, at which time the RHEED pattern will change from a featureless pattern to a streaked pattern representative of the GaAs crystal surface. The native oxide formed on GaAs has been found to desorb fairly abruptly from the sample surface at a temperature of 585°C, [16] therefore, by monitoring the RHEED pattern the desorption point of the native oxide can be used to calibrate the optical pyrometer used to measure the substrate temperature during growth.

2.3 Standard Sample Preparation.

The substrates used for this study were all commercially polished and oriented along the [100], [111A] or [111B] direction. Prior to introduction of the samples into the vacuum system, the wafers were prepared by using a 1,1,1-trichloroethane, acetone, methanol, and de-ionized (DI) water rinsing sequence. This involved rinsing the samples in an ultrasonically agitated bath of 1,1,1-trichloroethane for 30 seconds, followed by a similar 30 second rinsing in each of the other solvents listed. Following this rinsing, the samples were soaked in choline (Trimethyl (2-hydroxymethyl) ammonium hydroxide, (CH₃)₃N⁺CH₂CH₂OH·OH⁻, an alkaline solution which has been shown to provide extremely clean surfaces for epitaxial growth) for 1 hour. This procedure serves to remove any organic contaminants and particulate matter from the wafer surface. Subsequent to the choline soak, the samples were rinsed for 10 minutes in DI water, and then the spun dry to insure the maximum possible cleanliness was maintained. Samples
were then indium soldered to molybdenum blocks for material growth, at which time a thin native oxide was formed on the GaAs surface due to the heat used in the soldering process. Since a wafer with a (111A) oriented surface on one side will have a (111B) oriented surface on the opposite side, and vice versa, particular care was taken during the sample preparation of (111A) and (111B) oriented samples to ensure that samples were not flipped during the cleaning and mounting procedure. Subsequent to sample mounting, the growth blocks were introduced into the system through a vacuum interlock and placed on a heating stage where they were outgassed overnight before growth.

After the overnight outgassing procedure, Auger surface analysis was used to check the cleanliness of the sample surface, and then the sample was moved into the growth chamber where the substrate temperature was slowly raised using a resistively heated growth block heater. As discussed above, by monitoring the RHEED pattern during the heating procedure, the desorption of the native oxide from the GaAs surface at 585°C can be used to calibrate the optical pyrometer for subsequent temperature measurements during sample growth. After the pyrometer is calibrated, the substrate temperature is stabilized at 585°C, where a 5000Å buffer layer of undoped GaAs is grown. Since the epitaxial growth process tends to smooth out the surface over time and eliminate defects left by the mechanical polishing of the substrate material, this buffer layer improves the surface quality of the substrate substantially. After the completion of the buffer layer, the sample surface will be of sufficiently high quality that the desired experimental or device structure can be grown with minimal crystal defects due to substrate imperfections. Subsequent to the growth of the desired structure on the buffer
layer, the sample is removed from the growth chamber and Auger surface analysis is used to check the sample surface for cleanliness. After the final Auger analysis, the sample is removed from the system and unmounted from the growth block in preparation for further processing or characterization of the sample.

2.4 Van der Pauw Hall Measurements.

Post growth characterization of the sample resistivity and mobility was performed using Van der Pauw Hall [17] measurements. After the completion of the growth, the samples were removed from the system and cleaved into ~5 x 5 mm pieces for the fabrication of van der Pauw Hall structures. Ohmic contacts were then made to the sample in the standard van der Pauw configuration shown in figure 2.1 on page 15 using an ultra fine tipped Antex soldering iron and an alloy of 10%Zn/90%In for p-type contacts or 10%Sn/90%In for n-type contacts. These contacts were then sintered for 5 minutes at 485°C in a forming gas ambient to facilitate ohmic contact formation.

The Hall test measurement facility used for these measurements consisted of an electromagnet capable of producing up to 8000 Gauss, a specially designed sample holder, and a small Dewar which can be used to cool the sample to liquid nitrogen temperature by immersion into liquid nitrogen. A Keithley model 220 programmable current source, and a model 181 nanovoltmeter interfaced through an IBM compatible PC were used for sample bias and voltage measurement. A specially made switch box was used to connect
FIGURE 2.1
Van der Pauw Hall test structure.

The van der Pauw method was used to determine the Hall mobility, since this method allows calculation of the sheet resistivity and Hall mobility of an arbitrarily shaped sample. It was demonstrated by van der Pauw that given a sample which is uniformly thick, singly connected and has sufficiently small contacts located on the periphery of the sample, an accurate resistivity can be determined for the sample regardless of the sample shape. [17] In addition to the determination of sample resistivity, the method can be extended to measure the Hall mobility. [18]

A typical van der Pauw sample geometry is shown above in figure 2.1. Resistivity is determined from such a structure by passing a known current through contacts A and B and measuring the resulting voltage at contacts C and D. Any offset voltage that might exist is accounted for by performing this measurement again with the polarity of the
current through contacts A and B reversed and averaging the two measurements. This procedure is repeated three more times by passing current through contacts C and D, A and C, and B and D and measuring the respective voltages at contacts A and B, B and D and A and C. Using these measurements the sample resistivity can be determined regardless of the sample geometry. The Hall mobility is determined using the diagonal contact pairs A,D and B,C. By passing a known current through contacts A and D and measuring the resulting voltage at contacts B and C and vice versa, and repeating the measurements with the opposite current polarity, an average voltage can be determined for the sample. When the sample is placed in a magnetic field oriented perpendicularly to the sample surface, this voltage represents the Hall voltage induced by the magnetic field, and in the absence of a magnetic field this voltage should ideally be zero. By performing this voltage measurement in no magnetic field, and in positive and negative magnetic fields of equal magnitude, the Hall voltage can be measured accurately. By combining the resistivity and Hall measurements, the majority carrier type, concentration and Hall mobility can be then be determined. For a detailed explanation of the measurement and analysis, the reader should refer to references [17] and [18].

2.5 Photoluminescence Characterization.

In photoluminescence, an optical source having an emission energy larger than the bandgap of the material to be characterized is used to illuminate the sample causing the generation of electron-hole pairs with energies greater than the bandgap. These carriers
then rapidly thermalize to various allowed states in the semiconductor (i.e. conduction band minima, valence band maxima, impurity levels, etc.), where they then can recombine. When the correct quantum mechanical conditions are satisfied, an electron can radiatively recombine with a hole by emitting a photon with an energy equal to the energy difference between the electron and hole states. By examining the radiative luminescence emitted by a sample as a function of energy, information about the band structure and energy levels present in the sample can be determined. Since crystal defects and impurities deep in the bandgap can greatly reduce the efficiency of radiative recombination, the relative brightness of luminescence peaks is also a good indicator of the material quality.

In heterostructures, the presence of bandgap discontinuities allows crystal structures to be designed where quantum confinement of carriers in the direction perpendicular to the
interface is possible. Using elementary quantum mechanics, it can be shown that quantum confined structures (i.e. square or triangular potential wells) cause discrete allowed energy levels to form. For example, in the classic quantum mechanics problem of an infinitely deep square potential well of width $a$ (figure 2.2a on page 17), the energy levels are given by

$$E = \frac{n^2 \hbar^2}{2ma^2} \quad [19].$$

The actual energy levels for square [20] or triangular [21] quantum wells with finite potential (figure 2.2b on page 17), usually must be solved using numerical methods since no closed form analytical solutions exist.

Radiative transitions can also occur between the discrete energy levels present in quantum confined structures. The luminescence peaks emitted from a quantum confined energy level usually have a very narrow full width at half maximum due to the modified two dimensional density of states. The relative brightness of luminescence from quantum structures is usually much higher than the luminescence from bulk semiconductor material for this same reason. However, the linewidth and intensity of the emitted light can be affected adversely by roughness at the heterointerfaces, poor material quality, or weak quantum confinement.

Since many nonradiative processes, such as phonon emission or absorption, are strongly temperature dependent and their effects are minimized at low temperatures, samples are usually cooled to temperatures lower than $\sim 25$K. In addition to reducing nonradiative effects, cooling the sample reduces the thermal noise ($\approx 4k_bT$) and allows observation of shallow transitions which may not be apparent at room temperature. For example, many donor and acceptor levels are only 5 to 30 meV from the respective band edge and would not be visible in a room temperature photoluminescence measurement.
The photoluminescence system at OSU consists of an American Laser Corporation argon ion laser with a peak emission of 40mW at 488nm. The samples are cooled to a temperature of approximately 20K with an Air Products closed cycle helium refrigeration system. This system consists of a cold finger where samples are mounted, a cryoshroud which can be evacuated to prevent condensation formation, and a temperature controller for monitoring and adjusting sample temperature. The cryoshroud contains optical ports to allow laser access to the sample. The laser is focused on the sample using an optical rail with appropriate mirrors and lenses. The emission from the sample is then focused into a Jarrel-Ash 0.5m monochromometer which is connected to a photomultiplier for light detection. The photomultiplier is cooled using liquid nitrogen to eliminate thermal noise and improve efficiency. Data is then gathered with a Leading Edge IBM compatible computer outfitted with an A/D conversion board. A 670Hz chopper and lock-in amplifier are used to reduce noise and improve measurement efficiency, and appropriate filters are used in the optical path to remove unwanted laser lines from the sample emission spectrum. Typical operating conditions are a sample temperature of 20K, laser power density of ~1W/cm², and a 1100V bias on the photomultiplier tube cooled to a temperature of -90°C.

3.1 The Use of Carbon as a Dopant in III-V Semiconductor Materials.

In the growth of III-V compound semiconductors by MBE, beryllium is the most common p-type impurity used. However, beryllium exhibits significant diffusion [22] and surface segregation [23] in GaAs, and both of these effects are detrimental to the performance of many devices. It would be desirable to find an alternative p-type dopant which does not have these problems. Recently, carbon has been investigated as a possible alternative to beryllium for p-type doping in GaAs. Research on carbon doping in the III-V semiconductors has demonstrated that in addition to having a high level of electrical activity, carbon also has a much lower diffusion coefficient than other p-type impurities such as beryllium and zinc. [24,25,26] Consequently, carbon appears to be a promising candidate for p-type doping in GaAs.

However, since carbon is a group IV element, it can exhibit amphoteric doping behavior, which gives rise to either a C_{As} substitutional acceptor or to a C_{Ga} substitutional donor. Silicon, another group IV dopant used in GaAs, has been shown to exhibit strong amphoteric behavior, and silicon doped GaAs can be either n-type or p-type depending upon growth conditions and substrate orientation. [27,28,29] For instance, silicon doped GaAs grown on (100) oriented substrates is n-type [29], silicon doped GaAs grown on (111A) [28] oriented substrates can be either n or p-type depending on the growth conditions used, and silicon doped GaAs grown on (110) oriented substrates has been shown to produce p-type material [29]. Due to the chemical similarity of carbon and
silicon, it might be expected that carbon would exhibit similar amphoteric behavior. To date, studies of carbon doping in GaAs have shown that carbon does not exhibit strong amphoteric behavior and predominantly forms the $C_{As}$ acceptor impurity in GaAs. However, carbon doping experiments on substrate orientations other than the (100) surface of GaAs have not been previously reported. It is the purpose of the first part of this work to investigate the properties of carbon doping on (100), (111A) and (111B) oriented substrate materials in order to ascertain how material properties are affected by growth on different substrate orientations.

Currently there are two methods which have been successfully used to incorporate carbon into GaAs in a controlled manner in solid source molecular beam epitaxy (MBE) systems. The first method is the use of a resistively heated graphite filament which has been shown to be capable of controlled carbon doping up to concentrations of $1 \times 10^{20}/\text{cm}^3$. [5]. The second method is the use of gaseous carbon-tetrabromide which can be effectively controlled by a precision leak valve and has been shown to be capable of obtaining controlled carbon doping approaching concentrations of $1 \times 10^{21}/\text{cm}^3$ in GaAs. [30] It is expected that the use of a heated filament source produces carbon clusters which may lead to undesirable material properties. Since such clusters are not emitted from a gaseous carbon-tetrabromide source and carbon-tetrabromide has been shown to be an extremely efficient [30] carbon doping source which is relatively simple to implement, the MBE system at Oregon State University has been fitted with a carbon-tetrabromide source which was used for all carbon doping in this work.
3.2 Experimental Techniques.

The samples in this study were all grown by solid source Molecular Beam Epitaxy (MBE) in a Perkin Elmer Phi-425B MBE system. Samples were prepared for growth using the standard cleaning, mounting, and outgassing procedures described in section 2.3. After the outgassing procedure, samples were introduced into the growth chamber where the substrate temperature was gradually raised to the desired growth temperature of 585°C. During the substrate heating process, the desorption point of the native oxide was used to calibrate the optical pyrometer as described in section 2.2. Once the substrate temperature had stabilized at the growth temperature, a 5000Å buffer layer of undoped GaAs was grown on the substrate. Subsequent to the completion of the buffer layer 0.25 to 0.5 µm of carbon doped GaAs was grown depending upon the doping level used in the layer (doped layers must be grown thick enough to ensure that depletion of carriers will not significantly affect the Hall measurements).

The growth conditions used were optimized to obtain high quality epitaxial growth on each particular substrate orientation. Typical growth conditions for growth on (100) oriented substrates were a substrate temperature of 585°C, a growth rate of 1 µm/hr, and an arsenic to gallium flux ratio of ~5:1. For the (111A) and (111B) substrate orientations, the same substrate temperature of 585°C was used, but a larger arsenic to gallium ratio of ~20:1 was needed to obtain good epitaxial crystal growth and surface morphology. The needed 20:1 arsenic to gallium flux ratio was obtained through a combination of an increase in the arsenic flux and a decrease in the growth rate to as low as 0.2 µm/hr.
After the completion of the growth, the samples were removed from the system and cleaved into ~5 x 5 mm pieces for the fabrication of van der Pauw Hall structures. Ohmic contacts were then made to the sample in the standard van der Pauw configuration discussed in section 2.4 using an ultra fine tipped Antex soldering iron and an alloy of 10%Zn/90%In. These contacts were then sintered for 5 minutes at 485°C in a forming gas ambient to facilitate ohmic contact formation.

3.3 Hall Mobility Measurement Results.

The Van-der-Pauw Hall measurements showed that all the carbon doped samples exhibited only p-type conductivity regardless of the samples orientation. Furthermore, the carbon doped samples had carrier mobilities which were comparable to those obtainable in beryllium doped material with similar doping concentration. Therefore, in contrast to silicon, it appears that carbon exhibits little or no amphoteric behavior and is an efficient acceptor on all surfaces.

<table>
<thead>
<tr>
<th>Sample-dopant</th>
<th>Meas Temp</th>
<th>(100) Substrate</th>
<th>(111A) Substrate</th>
<th>(111B) Substrate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Carrier Conc. (cm$^3$)</td>
<td>Mobility (cm$^2$/Vs)</td>
<td>Carrier Conc. (cm$^3$)</td>
</tr>
<tr>
<td>Sample 300K</td>
<td>300K</td>
<td>2.19E18</td>
<td>140</td>
<td>---</td>
</tr>
<tr>
<td>#1 - Be 77K</td>
<td>300K</td>
<td>2.81E18</td>
<td>102</td>
<td>---</td>
</tr>
<tr>
<td>Sample 300K</td>
<td>77K</td>
<td>3.80E18</td>
<td>104</td>
<td>---</td>
</tr>
<tr>
<td>#2 - C 4.42E18</td>
<td>77K</td>
<td>97</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Sample 300K</td>
<td>8.52E19</td>
<td>53</td>
<td>9.76E19</td>
<td>35</td>
</tr>
<tr>
<td>#3 - C 8.08E19</td>
<td>77K</td>
<td>76</td>
<td>9.47E19</td>
<td>49</td>
</tr>
</tbody>
</table>

Hall measurement results for differing sample orientations grown simultaneously.
A plot of carrier concentration versus the leak valve setting is shown in figure 3.1 for each substrate orientation. From this figure it can be seen that the leak valve setting provided a reproducible control of carbon doping up to a concentration of $\sim 1 \times 10^{20}$/cm$^3$. Within the range of experimental error, this figure would appear to indicate that there is little or no dependence of doping efficiency upon the orientation of the substrate. To investigate this more carefully a few samples were grown in pairs with a (100) control sample and either a (111A) or a (111B) sample mounted on the same growth block. The Hall measurement results from these samples are shown in table 3.1. In this table it can be seen that the samples using beryllium dopant show comparable levels of doping for each orientation. The carbon doped samples grown simultaneously on the (100) and (111A) oriented substrates show similar doping concentrations on each orientation. But the

![FIGURE 3.1](image)

**FIGURE 3.1**
Carbon doping concentration versus leak valve setting of the CBr$_4$ source.
carbon doped samples grown simultaneously on (111B) and (100) substrates show a markedly different behavior with an apparent increase in carrier concentration on the (111B) surface with respect to the (100) surface. This behavior may indicate that the doping efficiency of carbon is slightly greater on the (111B) surface than on the (100) surface, which is somewhat unexpected, since it seems more probable that the (111A) Ga terminated surface where As atoms are only weakly bonded, would be more likely to exhibit an increase in p-type doping efficiency. However, it should be cautioned that the growth conditions for this dual growth were optimized for good growth on the (111B) surface, where the growth of high quality material requires a much larger arsenic overpressure than is optimal for growth of high quality material on the (100) surface. Therefore, the apparent increase in doping efficiency on the (111B) surface which is seen in this sample pair, could also be due to a measurement artifact resulting from inhomogeneities in the (100) oriented sample. Since only a limited number of samples could be grown for this study, further experiments of this type will be needed to ascertain whether the apparent doping increase on the (111B) surface is a real effect or is due to the non-optimal growth conditions used for the (100) sample.

A plot of Hall mobility versus carrier concentration for all samples is shown in FIGURE 3.2. In FIGURE 3.2a the 300K mobilities are plotted for carbon doped samples grown on (100), (111A), and (111B) oriented material and for beryllium doped samples grown on (100) and (111B) oriented material. From this figure several important conclusions can be made. First, the carbon doped samples all have mobilities which are similar to those of beryllium doped samples, indicating that the use of carbon as a dopant
FIGURE 3.2
Mobility versus doping concentration on various substrate orientations for beryllium and carbon doping in GaAs. a) Measurement results at 300K b) Measurement results at 77K.
does not degrade mobility. Second, there is no clear dependence of mobility upon the substrate orientation which was used. Finally the general trend in mobility with increasing carrier concentration is in good agreement with those reported in the literature. A similar plot of Hall mobility versus carrier concentration at 77K is shown in figure 3.2b. This figure also shows that there is no clear dependence of mobility upon substrate orientation or dopant type, and the trend in mobility with increasing carrier concentration is again in good agreement with the literature.

3.4 Photoluminescence Measurement Results.

Photoluminescence results for different doping levels are shown for each substrate orientation and dopant in figures 3.3-3.6. In figure 3.3 the normalized PL spectra for carbon doped samples grown on (100) oriented substrates are shown for $N_a - N_d = 3.3 \times 10^{17}$, $4 \times 10^{18}$, and $8.5 \times 10^{19}$ /cm$^3$. From this figure it can be seen that the full width at half maximum (FWHM) of the carbon peak increases as the doping level increases. As doping levels become large, the impurity states and valence band merge to form bandtail states. The presence of these bandtail states in addition to the Fermi level moving in to the band, causes broadening of the PL peaks at high doping concentrations. In addition to the broadening observed in the PL peak of the sample doped at $N_a = 8.5 \times 10^{19}$ /cm$^3$, a high energy shoulder at 1.47 to 1.48 eV can clearly be seen.
Photoluminescence spectra from carbon doped GaAs grown on (100) oriented substrates for various doping levels.

In accordance with the work of Kim et. al. [31] we believe that this high energy shoulder is most likely due to a conduction band to light hole transition which only becomes prominent at very high doping concentrations. Due to the fact that the carbon doped layer is only 0.25 um thick in the highest doped sample ($N_A = 8.5 \times 10^{19}$ /cm$^3$), the GaAs donor bound exciton ($D^0,X$) transition at $\sim 1.51$eV arising from the undoped GaAs buffer layer is still observed in this spectrum. [32] The PL spectrum for the lowest doped sample in this figure ($N_a = 3.3 \times 10^{17}$ /cm$^3$) also contains two peaks. The peak at $\sim 1.49$ eV is believed to be due to the transition of a free electron from the conduction band to a neutral bound acceptor ($e-A^0$) and the peak at $\sim 1.5$eV is most likely due to a combination of the ($A^0,X$) and ($A^+,X$) acceptor bound exciton peaks, [32] which are still visible due to the light doping in this sample, but can not be resolved at this temperature. In figure 3.3 it
Photoluminescence spectra from carbon doped GaAs grown on (111A) oriented substrates for various doping levels.

It can also be seen that due to the doping induced bandgap narrowing, the PL peak energy decreases as the carbon doping level increases.

In figure 3.4 the PL spectra for carbon doped samples grown on (111A) oriented substrates are shown for $N_a = 2 \times 10^{17}$ and $9.8 \times 10^{19}$ /cm$^3$. In this figure the PL spectrum for the low doped sample again has two peaks. The peak at $\sim 1.51$eV is the normal GaAs donor bound exciton ($D^0, X$) and is still visible due to the light doping in this sample, while the other peak at $\sim 1.49$eV is due to the transition of a free electron from the conduction band to a neutral bound acceptor ($e^{-}A_0^0$) [32]. The PL spectrum for the high doped sample shows what appears to be two peaks at $\sim 1.45$ and 1.49 eV. We believe that this is due to a conduction band to heavy hole and a conduction band to light hole transition, where the light hole transition has become more pronounced due to the extremely high doping.
Photoluminescence spectra from carbon doped GaAs grown on (111B) oriented substrates for various doping levels.

concentration in this sample. In this figure the effects of bandtail state induced broadening and bandgap narrowing in the highly doped sample are clearly visible. The peak position of the conduction band to heavy hole transition in the PL spectrum of the high doped sample also agrees quite well with the peak position of this transition in the PL spectrum for the $8.5 \times 10^{19} \text{ cm}^{-3}$ doped sample for the (100) orientation shown in figure 3.3.

In figure 3.5 the PL spectra for carbon doped samples grown on (111B) oriented substrates are shown for $N_a = 3.6 \times 10^{18}, 1.2 \times 10^{19}$, and $3.9 \times 10^{19} \text{ cm}^{-3}$. In this figure spectra of the two highest doped samples show a transition at $\sim1.51$eV, which is due to the fact that these layers were thin ($\sim0.25$ to 0.5 um), allowing the GaAs free exciton transition arising from the undoped GaAs buffer layer to be observed. In this figure the concentration dependent broadening of the PL peaks is clearly observable. However, the
expected shift of the PL peak to lower energy at high doping levels is not observed in the 3.9 \times 10^{19} /\text{cm}^3 doped sample. The PL for this sample is very weak and appears to have a peak at \sim 1.49\text{eV}, which is at a much higher energy than would be expected from our other results. We believe that this may be due to a problem with the growth of this sample since this sample showed clear defects in morphology. With the exception of the high doped sample, the peak position and width of the PL spectra in this figure agree well with those shown in figures 3.3 and 3.4.

**FIGURE 3.6**
Photoluminescence spectra from beryllium doped GaAs grown on (111B) oriented substrates for various doping levels.
FIGURE 3.7

Photoluminescence peak position versus doping concentration for carbon and beryllium doped GaAs grown on various substrate orientations.

For comparison, figure 3.6 shows the PL spectra for beryllium doped samples grown on (111B) oriented substrates, for $N_a = 1.3 \times 10^{18}$, $3 \times 10^{18}$, and $2 \times 10^{19}$ /cm$^3$. In this figure dependence of the peak position upon doping level agrees well with the dependence observed in the carbon doped samples. The PL of the beryllium doped samples also exhibits the bandtail state induced broadening as doping levels increase.

In figure 3.7 the peak energy for each PL spectrum versus doping concentration is plotted. This figure clearly shows the decrease in PL peak energy as doping level increases. With the exception of the (111B) $3.9 \times 10^{19}$ /cm$^3$ carbon doped sample, the PL peak energy decreases in a fairly smooth manner from $\sim 1.485$eV at lower doping concentrations to $\sim 1.45$eV at $1.0 \times 10^{20}$ /cm$^3$. These results agree quite well with similar results shown in reference [26], where the PL peak energy versus concentration for carbon
doped samples from three different groups is plotted. In figure 3.7 it can also be seen that samples with similar doping concentrations appear to have similar PL peak energies regardless of which orientation substrate was used for the growth.

3.5 Conclusions

We have studied the effect of substrate orientation upon the material properties of MBE grown carbon doped GaAs. Samples were grown on (100), (111A), and (111B) orientated substrates with doping levels varying from approximately $10^{17}/\text{cm}^3$ to $10^{20}/\text{cm}^3$. Van der Pauw Hall measurements showed all samples were p-type regardless of substrate orientation, and the mobility measured in the carbon samples was found to be comparable to similar beryllium doped samples. Even though carbon is a group IV element and can theoretically induce either p or n type behavior depending upon the substitutional site the impurity occupies, we have found no substrate dependence or strong amphoteric behavior for carbon doping in GaAs. This is quite different from the strong amphoteric behavior of silicon which produces either n or p-type doping depending upon substrate orientation and growth conditions. At high carbon doping levels ($p>5 \times 10^{19}/\text{cm}^3$) the PL spectrum shows an additional peak which is believed to be associated with a transition from the conduction band to light hole valence band.
4. The Effect of Substrate Temperature on the Growth of InGaAs.

4.1 Growth and use of InGaAs in III-V Compound Semiconductors.

The material properties of InGaAs compared to GaAs, such as narrower band gap and higher carrier velocity, have made it an important material for use in optoelectronic devices and high speed transistors. Due to the importance of InGaAs in these areas, the InGaAs/GaAs and InGaAs/AlGaAs material systems have been widely studied. The growth by molecular beam epitaxy (MBE) of high quality InGaAs layers is complicated by several factors. The relatively large lattice mismatch of 7% between InAs and GaAs can lead to serious morphological flaws in the InGaAs crystal such as misfit dislocations and threading defects, even for relatively low In content. Indium also exhibits significant surface segregation and re-evaporation [33,34,35,36] during growth. In order to minimize the loss of indium due to evaporation, InGaAs is usually grown at temperatures of 520-530°C at which indium loss is insignificant. The low (520-530°C) temperatures necessary for the growth of InGaAs are well below the 590-600°C temperatures needed for the growth of high quality AlGaAs layers, which makes the growth of high quality AlGaAs/InGaAs interfaces very difficult.

Although there is a large lattice mismatch between InGaAs and GaAs, Matthews and Blakeslee [6,7,8] showed that high quality epitaxial material can be grown upon a substrate with a significantly different lattice constant, provided that the epitaxial layer is thin enough. These studies showed that for sufficiently thin layers, the energy due to the
lattice mismatch between materials can be absorbed as elastic strain in the layers, without mitigating the formation of misfit dislocations. Static equilibrium dictates that the stress in the substrate and the thin epitaxial layer must be equivalent. Due to the large 400-500um thickness of the substrate material as compared to the 0.01-0.05um thickness of the thin epitaxial layer, very little local strain is induced in the substrate material, and it is commonly assumed that all of the strain is present only in the thin epitaxial layer. Thus, if InGaAs layers are grown sufficiently thin, the energy due to lattice mismatch between InGaAs and GaAs or AlGaAs will be absorbed as strain in the InGaAs layer.

The strain in the InGaAs layer is produced by a reduction in the in-plane lattice constant of InGaAs to conform to the lattice constant of the GaAs substrate in the directions parallel to the interface as shown in figure 4.1. Since the strained lattice constant of the InGaAs conforms to the lattice constant of the substrate material, the material is referred to as pseudomorphic material. If the thickness of the InGaAs layer

![Figure 4.1](image)

**FIGURE 4.1**
Schematic showing effect of biaxial strain in pseudomorphic InGaAs.
becomes too large, the formation of misfit dislocations becomes favorable, and the lattice constant of the InGaAs will relax to its unstrained value via dislocation formation. The critical thickness at which a layer of In$_y$Ga$_{1-y}$As will relax back to its native lattice constant is dependent on the mole fraction, $Y$, of indium present in the layer. Since the mismatch and strain in a In$_y$Ga$_{1-y}$As layer increase as the mole fraction $Y$ of indium increases, the critical thickness for misfit formation decreases with increasing indium composition. Based on the work of Anderson [37], a curve showing the dependence of critical thickness upon indium mole fraction is shown in figure 4.2.

The growth of high quality structures containing InGaAs layers is further complicated by the large difference in substrate temperatures necessary to grow InGaAs, GaAs and AlGaAs. Even when InGaAs layers are grown with thicknesses less than the critical thickness, indium atoms are sufficiently mobile at the growth temperature that
significant segregation and re-evaporation occurs. To minimize these effects InGaAs layers are commonly grown at temperatures of 530°C or below where indium re-evaporation is negligible and the indium segregation rate is low. The surface mobility of gallium at such low substrate temperatures; however, is so low that a large number of native defects are incorporated into the crystal. These defects can lead to a large density of mid-gap states and a high excess carrier recombination rate, properties which are undesirable for most semiconductor device operation. To minimize the formation of these type of defects, GaAs is typically grown at temperatures near 580°C, at which gallium has a large surface mobility and can easily form relatively defect free layers. Due to the fact that aluminum forms stronger bonds with arsenic than either gallium or indium, the optimal growth temperature for AlGaAs layers is even higher than for GaAs layers. The optimal growth temperature for AlGaAs with high quality electrical characteristics (i.e. AlGaAs layers in MODFET structures) is near 610°C and for AlGaAs which has both high quality optical and electrical characteristics (i.e. AlGaAs cladding layers in laser diodes) is near 680°C.

Growth interruptions after the completion of an InGaAs layer may also be used to raise the substrate temperature for the subsequent growth of GaAs or AlGaAs layers. In some cases the use of such an interruption has been shown to improve the InGaAs interface by allowing excess surface indium to re-evaporate and the surface of the InGaAs layer to smooth out. [38,39] However, it has also been suggested that excessive loss of indium from the InGaAs layer may occur, causing degradation of the interface, when the growth interruption is too long. [43] Since indium segregation and reevaporation are
highly temperature dependent and increase dramatically at high temperatures, it is important to assess carefully the effects of growth interruptions upon the quality of InGaAs grown at high temperatures.

Due to the complications which this large disparity in optimal growth temperatures creates in the growth of InGaAs/GaAs and especially InGaAs/AlGaAs interfaces, the growth of InGaAs at higher temperatures has been investigated. These studies have reported that both segregation and re-evaporation of indium increase dramatically with the increase of the growth temperature. [40,41,42,43] Although indium segregation and reevaporation appear to have a dramatic temperature dependence, very few studies of the growth of InGaAs at higher temperatures have been done and the physics of InGaAs growth at high temperatures is not well understood.

Because of the possible benefits of growing InGaAs at temperatures near 580-600°C where GaAs and AlGaAs can be grown more readily, the mechanisms of InGaAs growth as a function of temperature were studied using reflection high energy electron diffraction (RHEED), Auger Electron Spectroscopy and photoluminescence (PL) measurements. The effect of temperature and growth interruptions upon the growth of InGaAs were characterized by measuring the intensity of the elastically scattered specular spot in RHEED measurements during growth. These measurements highlighted new features in the growth of InGaAs which are not directly apparent in the observation of the RHEED patterns themselves. The significance of these new features in the RHEED intensity oscillation measurements was further studied by growing several GaAs/In_{0.2}Ga_{0.8}As/GaAs and GaAs/In_{0.2}Ga_{0.8}As/Al_{0.2}Ga_{0.8}As single quantum well
structures for PL measurements. These experiments show that the linewidth of the PL is narrowest in samples grown at a temperature of 575°C without growth interruption. Results also indicate that the use of growth interruptions at the end of an InGaAs layer may be detrimental to the quality of the interface and that prolonged growth interruptions may even lead to a loss of indium from the bulk of the InGaAs quantum well. Further experiments are in progress to assess the magnitude and significance of indium loss during growth interruptions.

4.2 Experimental Technique.

The epitaxial layers used for this study were grown in a Perkin Elmer 425B MBE system on GaAs samples indium soldered to molybdenum blocks. The arsenic flux (As₂) from a standard solid source oven with a cracker was adjusted so the V/III beam equivalent pressure ratio was always above seven as determined by a quadrupole mass spectrometer in direct line of sight with source ovens. As described in section 2.2, RHEED intensity oscillations were used in all cases to calibrate the gallium, indium and aluminum metal fluxes. The calibration procedure consisted of adjusting the temperature of one of the Ga source ovens to 0.8 monolayer/s growth rate, while the other Ga oven and the indium and aluminum ovens were set to temperatures to provide a growth rate of 0.2 monolayer/s each. Thus In₀.₂Ga₀.₈As, Al₀.₂Ga₀.₈As, and GaAs could all be grown at a nominal growth rate of 1.0 monolayer/s. The nominal indium growth rate of 0.2 monolayer/s was calibrated at a substrate temperature of 550°C.
Due to the large dependence of indium incorporation upon substrate temperature, the actual incorporation of indium will be larger at lower substrate temperatures. Thus, if the indium composition and layer thickness are not carefully chosen, InGaAs layers grown at higher temperatures might be pseudomorphic and contain relatively few defects, while InGaAs layers grown at lower substrate temperatures might exceed the critical thickness for pseudomorphic growth and contain many defects due to the increased indium incorporation. Because of this, the InGaAs layer thicknesses and nominal indium composition were chosen to allow pseudomorphic InGaAs layers to be grown at all substrate temperatures used in this study.

The substrates used for this study were all commercially polished and oriented along the [100] direction. Samples were prepared for growth using the standard cleaning, mounting, and outgassing procedures described in section 2.3. After the outgassing procedure, samples were introduced into the growth chamber where the substrate temperature was gradually raised to the desired growth temperature of 585°C. During the substrate heating process, the desorption point of the native oxide was used to calibrate the optical pyrometer as described in section 2.2. Once the substrate temperature had stabilized at the growth temperature, a 5000Å buffer layer of undoped GaAs was grown on the substrate.

After the growth of the buffer layer, the substrates were used either to examine the behavior of RHEED oscillations upon various growth conditions, or for the growth of single InGaAs quantum wells for photoluminescence (PL). For the RHEED experiments, the intensity of the specular RHEED spot was monitored as a function of time by using an
optical fiber to couple the intensity of the RHEED spot into a photomultiplier tube. The output of the photomultiplier tube as a function of time was then measured using a digital storage oscilloscope. Since the growth of InGaAs causes surface roughening and increased strain in the crystal, after each RHEED oscillation experiment involving an InGaAs layer, a short buffer of GaAs was grown to improve the crystals quality, ensuring that subsequent InGaAs layers could be grown pseudomorphically. The InGaAs layers grown for photoluminescence measurements consisted of 5000Å/85Å/1000Å GaAs/In_{0.2}Ga_{0.8}As/GaAs single quantum wells grown at 520°C, 575°C and 595°C with and without a 30 second growth interruption after the completion of the InGaAs quantum well. Photoluminescence measurements were made at 20K with excitation provided by the 548nm line from an Ar+ laser at a typical density of ~1W/cm^2. The PL signal from the sample was detected by a liquid nitrogen cooled photomultiplier tube with Si cathode and a lock-in amplifier. The reference signal for the lock-in amplifier was provided by the output of the 670 Hz beam chopper used to chop the incident laser beam.

4.3 Experimental Results and Discussion.

Fig. 4.3 shows the specular spot intensity variation vs. time for several substrate temperatures. All curves start at time 0 when In and Ga shutters are opened and In_{0.2}Ga_{0.8}As (nominal composition) is grown for 20 seconds. After 20 seconds the In
FIGURE 4.3
RHEED oscillation intensity versus time for various substrate temperatures.

shutter is closed and the other Ga shutter is opened to continue the growth of GaAs at the nominal growth rate of 1 monolayer per second. As it can be seen from the figure 4.3 a dramatic change in the intensity behavior occurs when the substrate temperature is changed from 564°C to 567°C. For substrate temperatures 564°C and below the closure of the In shutter causes a slow and steady increase of the specular spot intensity; whereas for higher substrate temperatures (567°C and above) we observe little change in the intensity of the signal for a period of time after the In shutter gets closed, and then a sharp increase followed by recurring oscillations.

By observing the actual RHEED pattern above and below 565°C we find that for substrate temperatures above ~567°C the surface reconstruction pattern changes from a
(2x4) arsenic-stabilized pattern to a (4x2) metal-stabilized pattern a few seconds after the start of InGaAs growth. The surface remains in the (4x2) reconstruction during the remainder of the InGaAs growth and does not change back to the (2x4) arsenic stabilized pattern until some time after the indium flux is shut off. This change back to the (2x4) pattern is fairly abrupt and coincides with the sharp increase of specular spot intensity seen in all but the bottom curve of figure 4.3.

For substrate temperatures below ~565°C (Fig. 4.3, bottom curve) the reconstruction pattern dims into a relatively featureless background several seconds after the start of InGaAs growth. This pattern persists throughout the growth of the InGaAs layer until the In shutter is closed and the pattern begins to slowly recover from this dim featureless background to the usual (2x4) pattern during the subsequent GaAs growth. At these lower temperatures all transitions in RHEED patterns were gradual and no abrupt phase transitions in the RHEED pattern, similar to those observed at higher temperatures, were seen.

Indium induced (4x2) surface reconstruction during the growth of InGaAs has been observed before [40,41] but our experiments demonstrate how sharp and temperature sensitive the transition from arsenic stabilized to metal stabilized is. A change of just 3°C is enough to induce this phase transformation. The substrate temperature at which this transition occurs is a function of the As flux and, as would be expected, as the As flux increases the temperature of the substrate at which this transition occurs also increases. It can also be seen in figure 4.3, that the time it takes for the reconstruction pattern to switch back to (2x4) As stabilized is a function of substrate temperature; the
higher the temperature the shorter is the time. Similar observation has been made by Woodbridge. [41]

As the temperature of the substrate is increased, the amount of indium segregating to the surface increases and at some point in time after the start of InGaAs growth the surface concentration of indium is such that a transition to a metal stabilized diffraction pattern occurs. After the indium shutter is closed, the surface will remain in the metal rich (4x2) reconstruction for a time and then it will switch abruptly back to a (2x4) arsenic stabilized reconstruction. We believe that the time between the closing of the indium shutter and the transition from metal rich to arsenic stabilized surface reconstruction, is the time necessary for the excess indium to evaporate from the surface. As substrate temperature is increased, the evaporation of indium is significantly increased and thus, this transition time will be decreased, as can be seen from the RHEED intensity behavior in figure 4.3. From figure 4.3, the time from the closing of the In shutter to the sharp increase in RHEED intensity, \( t_r \), can be calculated for each substrate temperature. An Arrhenius plot of \( \ln(1/t_r) \) versus \( 1/T_{SUB} \), where \( T_{SUB} \) is the substrate temperature in K, can then be made to determine the activation energy for this process. The resulting activation energy calculated from the data in figure 4.3 is found to be \( E_A = 1.845 \) eV. This value corresponds well with the reported values of 1-3 eV for the activation energy for indium desorption from the (100) GaAs surface[44]. It is important to note that at temperatures above this transition temperature, the incorporation of In (and probably to some extent Ga as well) is As flux limited, as is always the case for growth under metal rich conditions. One can assume that it is the incorporation of indium atoms that will be affected the most.
since In forms a weaker bond with As as compared to Ga or Al. This fact can make it difficult to grow material with a particular In concentration reproducibly because not only In but As flux needs to be calibrated as well.

The other problem with the growth under metal rich conditions is that, as can be seen from figure 4.3, the surface remains metal rich for a period of time after the In shutter is closed. This is presumably caused by excess indium at the surface. Thus, when one proceeds without interruption with the growth of GaAs, some of this excess In gets incorporated into the lattice and smears out the heterointerface.

One of the objectives of this work was to examine the effects of a growth interruption at the end of the growth of an InGaAs quantum well. In principle, this
interruption can be used to allow the reevaporation of excess indium and smoothing of the InGaAs interface. [38,39] In the case where the barrier is to be AlGaAs, the growth interruption also allows growth temperature to be increased to improve the quality of the AlGaAs.

Figure 4.4 shows two curves of RHEED intensity versus time for growth at 590°C. Again, both curves start at time 0 when In and Ga shutters are opened and In$_{0.2}$Ga$_{0.8}$As is grown for 20 seconds. At time 20 seconds after the start of InGaAs growth, either both the In and Ga shutters are closed (bottom curve) or only the In shutter is closed and simultaneously a second Ga shutter is opened (top curve). Stopping the growth and annealing in As flux (bottom curve) produces a sharp short drop and then slow and gradual increase of the specular spot intensity. As it can be seen from figure 4.4, the RHEED signal recovery time is shorter when there is a total growth stop, thus it would appear that the heterointerface might be improved through the use of a short growth interruption after the completion of an InGaAs layer.

To investigate the effect of a stop growth on the quality of InGaAs interfaces we examined the PL spectra from 5000Å/85Å/1000Å GaAs/In$_{0.2}$Ga$_{0.8}$As/GaAs single quantum wells grown at 520°C, 575°C and 595°C with and without a 30 second growth interruption after the completion of the InGaAs quantum well. The PL peak position and full width at half maximum (FWHM) for the samples are shown in Table 4.1. In this table it can be seen that the PL FWHM was significantly larger when a stop growth was used. The broadening of the PL FWHM when a stop growth was used was also observed by
TABLE 4.1
PL peak position, full width at half maximum, and In composition for InGaAs samples grown at different temperatures.

<table>
<thead>
<tr>
<th>PL Sample Structure</th>
<th>Growth Temp.</th>
<th>No stop growth</th>
<th>With stop growth</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>PL Peak Position</td>
<td>FWHM</td>
</tr>
<tr>
<td>GaAs/InGaAs/GaAs</td>
<td>595°C</td>
<td>1.47eV</td>
<td>4meV</td>
</tr>
<tr>
<td>5000Å/85Å/1000Å</td>
<td>575°C</td>
<td>1.360eV</td>
<td>4meV</td>
</tr>
<tr>
<td></td>
<td>520°C</td>
<td>1.283eV</td>
<td>7meV</td>
</tr>
<tr>
<td>GaAs/InGaAs/AlGaAs</td>
<td>595°C</td>
<td>no In</td>
<td>no In</td>
</tr>
<tr>
<td>5000Å/85Å/1000Å</td>
<td>575°C</td>
<td>1.340eV</td>
<td>14meV</td>
</tr>
<tr>
<td></td>
<td>520°C</td>
<td>1.299eV</td>
<td>12meV</td>
</tr>
<tr>
<td>GaAs/InGaAs/GaAs/AlGaAs</td>
<td>575°C</td>
<td>1.355eV</td>
<td>7meV</td>
</tr>
</tbody>
</table>

Nagle et. al. [39] who ascribed it to surface roughening caused by continued reevaporation of indium.

We also observe a shift toward higher energy of the PL indium related peak from the samples with a growth interruption as compared to the uninterrupted growth samples. The broadening of the well caused by incorporation of an extra In from the accumulation layer in the case of the uninterrupted growth would lower the ground state leading to a similar shift in PL. However, the shift we observe is too large to account for by broadening of the well alone. Thus, this shift seems to indicate that growth interruptions can lead to an increased loss of indium from the bulk of the well. We speculate that the interface degradation and higher indium losses from growth interruption are caused by an enhanced bulk diffusion of indium to the surface. This enhanced bulk diffusion occurs presumably because reevaporation of surface indium leaves vacancies behind and these vacancies promote diffusion of indium atoms to the top where they evaporate with vacancies left behind and so on.
Some additional confirmation of the importance of indium bulk out-diffusion is obtained from a second set of quantum well samples where an outer $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ barrier instead of GaAs was grown. The samples from this set grown at 595°C with or without growth interruption do not show any indium at all in PL spectra. While the lack of an indium related peak in PL spectrum does not rule out the presence of indium, this is consistent with the results of Radulescu et al. [40] who studied indium incorporation using Auger depth profiling and detected no indium at the intended InGaAs quantum well position in samples with AlGaAs barriers grown at 590°C. These results indicate that aluminum atoms seem to promote indium segregation. This can be rationalized by recognizing that aluminum makes a stronger bond with As than gallium and gallium makes a stronger bond with As than In. Thus, the incoming Al atoms would tend to displace In atoms from the crystal surface, where they could easily reevaporate and create vacancies which would enhance the diffusion of In atoms coming to the surface from the bulk.

Our other samples with top $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ barrier grown at lower substrate temperature than 595°C do show In related peaks in PL spectra (see Figure 4.5). As expected, the PL peaks related to indium move progressively toward higher energies as the temperature at which the samples were grown is increased. In general, our PL data confirm that it is difficult to control the loss of indium when the growth of InGaAs layers is under metal rich conditions, that is, when metal incorporation is As flux limited.
FIGURE 4.5
Photoluminescence spectra for 85Å InGaAs quantum wells with one AlGaAs barrier layer. Growth temperatures 520, 575 and 595°C. Sensitivity 100x at 520°C. Also shown is the result for a well with a 50Å GaAs spacer between the InGaAs and the AlGaAs.

The PL peak positions from InGaAs/AlGaAs and InGaAs/GaAs samples grown under identical conditions are fairly close to each other indicating that the indium incorporation is similar in both types of samples. However, as it can be seen in figure 4.5, the peak from samples with an AlGaAs barrier is either very dim, as for the sample grown at 520°C, or fairly broad, as for the sample grown at 575°C. These results indicate a higher roughness of InGaAs/AlGaAs interfaces as compared to InGaAs/GaAs interfaces. In an effort to minimize the enhanced segregation of indium caused by the presence of aluminum atoms we have grown samples with a 50Å GaAs spacer between the InGaAs and AlGaAs. This approach is similar to the one reported by Kraus et. al. [45] who
inserted thin 4 monolayer GaAs spacers between InGaAs and AlGaAs in their heterostructure field effect transistors. As can be seen in figure 4.5, the sample with the GaAs spacer has a much narrower FWHM than any of the other aluminum containing samples and has a peak energy which indicates an indium incorporation of ~17%. From a device application point of view, these results suggest that problems with making quality heterostructure InGaAs/AlGaAs devices may be alleviated by growth at higher temperatures and with the addition of a GaAs buffer before the AlGaAs.

Post growth Auger spectra from the GaAs/InGaAs/GaAs and GaAs/InGaAs/AlGaAs samples showed that there was 0.2-2% indium concentration present at the sample surface in all of these samples even though 1000Å of material (GaAs or AlGaAs) was grown on top of the InGaAs quantum well. Surface concentrations of indium were between 1 to 2% in samples without a stop growth, while they were about 10 times less (~0.2%) in samples with a growth interruption. The presence of indium on the surface of samples in spite of the growth of 1000Å of either GaAs or AlGaAs on top of the InGaAs quantum well suggests two possibilities. The first possibility is that a small amount of indium continues to diffuse to the growth surface from the bulk of the InGaAs quantum well by means of vacancy diffusion. However, this seems highly unlikely, since incorporation of indium uniformly throughout the bulk of a 1000Å layer of GaAs or AlGaAs even at the levels of 0.2-2% would consume a substantial portion of the indium contained in an 85Å In0.2Ga0.8As quantum well, causing severe degradation of the quantum well, and PL from the samples indicates that the growths produced high quality InGaAs quantum wells which contain reasonable amounts of indium. The other
possibility, which seems more plausible, is that below a certain level indium will not readily incorporate into the growing crystal, and thus segregation forces a small amount of indium to flow along with the growth surface thereby leaving a trace amount of indium present at the surface of the 1000Å GaAs or AlGaAs overlayer without causing significant indium to be incorporated into the bulk of the overlayer. In order to determine more about this effect, either Auger or SIMS depth profiling of the samples is necessary to determine whether indium is present only at the surface of these samples or is present throughout the bulk of the overlayer. Unfortunately, at the time of this work, neither Auger or SIMS profiles could be obtained to investigate this effect. It is suggested that these experiments would be a good area of future work which might shed some valuable insight on this effect.

Although our results indicate that the use of 30 second growth interruptions may cause serious degradation of the InGaAs/GaAs and InGaAs/AlGaAs interfaces and may lead to loss of indium from the quantum well itself, it cannot be excluded that growth interruption can still be of value. Other groups have indicated that much shorter [38,46] growth interruptions than the 30 second interruptions we used, or growth interruptions applied not directly after completion of InGaAs layer but rather after capping it first with several GaAs layers [39] may lead to an improvement of InGaAs material quality.
4.4 Conclusions.

We have found the bulk inter-diffusion process to be an important factor in physics of the InGaAs/GaAs interface and even more so in InGaAs/AlGaAs interface. The increased indium reevaporation at about 565°C coincides with the phase transition of the surface reconstruction from As stabilized to metal stabilized and it is caused by arsenic limited incorporation of indium. We have found that the quality of InGaAs/AlGaAs materials can be greatly improved by growing the layers at relatively high substrate temperature and inserting a GaAs spacer between the two layers. Finally, we have found a small amount of indium present on the surface of samples even though a 1000Å overlayer of GaAs or AlGaAs was grown on the InGaAs quantum well. This result may indicate that either bulk outdiffusion from the InGaAs quantum well or segregation of a small surface layer of indium occurs during overlayer growth; however, more experiments are needed to understand this phenomenon fully.

5.1 History of GaAs Grown at Low Temperatures and Experimental Background.

Normally, molecular beam epitaxy (MBE) uses growth temperatures between 580-600°C to grow high quality GaAs layers. However, in 1988, Smith, Calawa and coworkers discovered that GaAs grown at relatively low temperature near ~200°C (LT-GaAs) had many unusual properties, and was ideally suited for buffer layers to prevent backgating in GaAs MESFETs. [11] Since this discovery, LT-GaAs has been widely studied and has shown promise for use in many devices. In 1993, a two day symposium on LT-GaAs and related materials was held, and 31 of these papers were subsequently published in a special issue of the Journal of Electronic Materials [47] devoted to the topic of LT-GaAs. This reference is suggested as a good synopsis of work in this area up to that time and would be a good starting point for someone interested in the details of LT-GaAs. A brief summary of both the general results published in this issue of the Journal of Electronic Materials and the current status of research in the area of LT-GaAs is presented here.

As grown LT-GaAs has been shown to be non-stoichiometric with an arsenic excess on the order of 1% [9] and is moderately conductive. Reflection high-energy electron diffraction (RHEED) and double-crystal x-ray diffraction data indicate that this material is still highly crystalline. [11] However, the excess arsenic in this material forms a large number of As antisite point defects and causes the lattice constant to increase by ~0.1%. [10,48] Upon annealing at temperatures near 600°C, the excess arsenic in the
material precipitates out to form small clusters, the lattice constant becomes the same as
for that of bulk GaAs, and the material becomes highly resistive. [10] Further
measurements have shown that even when doped with silicon at levels greater than
$1 \times 10^{18}/\text{cm}^3$, this material remains semi-insulating after a 600°C anneal. [10] The high
resistivity of this material makes it ideal for use as an insulating buffer layer for devices
such as modulation doped field effect transistors (MODFETs) and metal semiconductor
field effect transistors (MESFETS). [11,12]

The excess carrier recombination lifetime in LT-GaAs is extremely short (~1ps),
[13,14] and the recombination process in LT-GaAs is found to be predominantly
nonradiative, since no photoluminescence (PL) was observed in initial studies of the
material. [10] However, more recent studies have reported weak PL lines arising from hot
carriers injected by picosecond excitation, [49] and a large number of sharp lines arising
from arsenic interstitial (As$_i$) related defects and their phonon replicas. [50,51] The
extremely short carrier lifetime, predominantly non-radiative recombination and large
resistivity of LT-GaAs makes it ideally suited for high speed photodetector applications.
P-i-N photodetectors using LT-GaAs for the i-region have demonstrated both low dark
currents and photoresponse faster than 2Ghz. [52] These detectors have also shown a
significant responsivity in the 1.3 to 1.5 μm range [52], which is well below the normal
bandgap of GaAs. This sub-bandgap response is thought to be due to internal
photoemission from the arsenic clusters present in annealed LT-GaAs layers. Metal-
semiconductor-metal (MSM) photodetectors fabricated on bulk layers of LT-GaAs,
similarly to LT-GaAs P-i-N photodetectors, exhibit significant sub-bandgap response and
low dark currents, and an extremely fast response time on the order of a few picoseconds. [52,53]

Although the unusual properties of LT-GaAs make it well suited for many device applications, many of the intrinsic material properties of LT-GaAs have not yet been well characterized. The extremely large resistivity of annealed LT-GaAs makes it very difficult to study the transport properties of this material by conventional experimental techniques such as Hall effect measurements. Due to this difficulty there has been only limited progress in understanding the transport properties of LT-GaAs. In spite of this, research on LT-GaAs transport properties has established that conduction in thick (~1μm) single layers of LT-GaAs can occur via two possible mechanisms. [54,55] The first mechanism is conduction through the delocalized band states, and the second mechanism is hopping conduction through defect states. The relative importance of each of these mechanisms seems to be determined by both the measurement temperature and the sample history (growth temperature, annealing conditions, etc.).

This work presents the first study of the Hall mobility of a two-dimensional electron gas (2-DEG) in MBE-grown LT GaAs using a novel MODFET device structure in which the channel region is made of LT-GaAs and all other layers are grown at normal temperatures. In the dark, the resistivity of this material is found to be extremely large, just as in bulk layers of LT-GaAs. However, when this new structure is illuminated, its resistivity becomes significantly lower than that of single layers of LT-GaAs, allowing reliable Hall measurements to be performed even at temperatures as low as 77K. To understand the significance of the Hall measurements more fully, theoretical values of the
low field mobility of a 2-DEG in LT-GaAs were calculated from the solution of the Boltzmann equation under a relaxation time approximation by taking into account the relevant scattering mechanisms. A first order approximation for the scattering due to the presence of arsenic clusters in the LT-GaAs was implemented for the first time in this calculation. The results of this calculation are found to be in good agreement with experimental results.

Although only weak photoluminescence has been observed previously in bulk layers of LT-GaAs, the results of PL measurements performed at 25K on this novel LT-GaAs MODFET structure show a new PL line at 1.65eV. The position of this new PL feature is at an energy which is significantly larger than the bandgap of GaAs and significantly lower than the bandgap of the AlGaAs barrier layers used in this structure. It is proposed that this PL line arises from a spatially indirect transition from a two-dimensional electron gas in the LT-GaAs at the heterojunction interface to the holes generated in the AlGaAs barrier layers.

Due to the extremely large light sensitivity of the LT-GaAs MODFET structure, photodetectors with an interdigital pattern of Ni/AuGe/Au ohmic metalization were fabricated on this structure. These detectors exhibited an excellent responsivity of 65A/W at ~0.87μm and 6.5A/W at ~1.0μm. These values of responsivity are among the highest reported for any GaAs based photodetector, and indicate that this device may be promising for applications requiring high sensitivity, especially in the 1.3 μm range. Present results indicate that the speed of these devices is much lower than that of the LT-GaAs P-i-N photodetectors and Schottky barrier MSM photodetectors fabricated on bulk
LT-GaAs. Work is ongoing to improve the speed response of these devices and/or find an application suited to the high sensitivity and lower speed currently exhibited by these detectors.

5.2 Growth of LT-GaAs MODFET Structure

Many of the growth procedures used in the fabrication of device structures by MBE are fairly similar. Although the growth details of normal GaAs/AlGaAs MODFET structures have been reported widely in the literature, the use of GaAs grown at low temperatures in the channel region of these structures has not been previously attempted. The use of LT-GaAs in these structures requires a significantly different growth procedure than that used for the growth of normal MODFETs. In this section the growth procedure used for the novel LT-MODFET structure will be discussed in some detail.

The LT-GaAs MODFET structures were grown in a PHI 425B Molecular Beam Epitaxy system. Growth rates were calibrated to a nominal rate of 1.0 monolayer/second using reflection high energy electron diffraction (RHEED) oscillations as described in chapter 2.2. The substrate temperature was measured using an optical pyrometer calibrated to the desorption of the native oxide at 585°C and with a thermocouple for temperatures lower than ~400°C for temperatures out of the range of our pyrometer. Surface quality and cleanliness was checked both before and after material growth using an in-situ Auger electron analyzer.
The samples were all grown on (100) LEC GaAs substrates. Samples were prepared for growth using the standard cleaning, mounting, and outgassing procedures described in section 2.3. After the outgassing procedure described in section 2.3, samples were introduced into the growth chamber where the substrate temperature was gradually raised to a growth temperature of 585°C using a resistively heated growth block heater. During the substrate heating process, the desorption point of the native oxide was used to calibrate the optical pyrometer as described in section 2.2. Once the substrate temperature had stabilized at 585°C, a 5000Å buffer layer of undoped GaAs was grown on the substrate. Then, the growth was stopped by closing the gallium shutters while the arsenic shutter remained open. The substrate temperature was then lowered to 250-350°C for the growth of the LT-GaAs layer. After the substrate temperature had stabilized at the desired temperature, 5000Å of undoped LT-GaAs was grown. After the completion of the 5000Å LT-GaAs layer, the growth was again stopped and the substrate temperature raised to 585°C for the growth of the remaining layers. Once the substrate temperature stabilized at 585°C, 150Å of undoped Al_{0.2}Ga_{0.8}As, 350Å of 1x10^{18}/cm^3 silicon doped Al_{0.2}Ga_{0.8}As and 200Å of 1x10^{18}/cm^3 silicon doped GaAs were grown. In some samples a thin 65Å layer of undoped GaAs was grown at 585°C between the LT-GaAs layer and the 150Å undoped Al_{0.2}Ga_{0.8}As layer. The growth of the high temperature MODFET layers also served to anneal the LT-GaAs layer. The arsenic flux was maintained at growth levels during all stop growths.
5.3 Device structure and principle of operation.

A standard MODFET consists of four basic layers, the active layer or channel, the spacer layer, the barrier and doping layers, and the cap layer (see figure 5.1). The active region of a MODFET is undoped. A heavily doped material of larger bandgap is then grown upon the active region. Due to the discontinuity in charge present at the heterointerface, carriers transfer from the doped side into the active region in order to align the Fermi level across the heterojunction in equilibrium. The result is a charge accumulation layer near the heterointerface as was first predicted by Anderson.[56] The ionized impurities in the doped layer and the charge in the active region create large internal electric fields, and pronounced band bending occurs. This large band bending in conjunction with the bandgap discontinuity produces a potential well at the heterointerface, resulting in quantum mechanical size confinement of carriers. The quantum confinement causes the formation of discrete energy levels which the carriers occupy. This confines the charge in the active layer to a region which is only a few tens of angstroms in width in the direction perpendicular to the heterointerface, while the charge carriers are free to move in the two dimensions parallel to the interface. The carriers in the well are thus described as a two dimensional electron gas (2-DEG).

In a normal MODFET, since the channel region is undoped and the charge is well confined in this region, scattering due to impurities is greatly reduced and large carrier mobilities can be achieved. This mobility enhancement is much more pronounced at low temperatures where ionized impurity scattering is a dominant factor limiting carrier...
mobility. As predicted by Esaki and Tsu[57], the addition of a spacer layer of undoped material between the doping and the active region will increase the mobility of the carriers in the active region. This increase occurs due to the physical separation of the parent impurity atom and carrier, which reduces the strength of the scattering potential. This enhanced mobility was first shown by Dingle et. al.[58] for electrons in a AlGaAs/GaAs heterostructure. Later Störmer and Tsang[59] demonstrated a similar mobility enhancement for holes in a AlGaAs/GaAs heterostructure.

FIGURE 5.1
Schematic cross-section of a LT-MODFET structure.
The novel MODFET structure used in this work is shown in Figure 5.1 on the previous page. The structure is essentially that of a normal MODFET in which the channel region is made from LT GaAs. The structure differs from other MODFET structures which have used LT-GaAs buffer layers to reduce backgating in that the LT-GaAs in this device extends right up to the heterojunction interface (or within 65Å of the interface in some devices).

The principle of operation of the new LT-GaAs MODFET device is similar to the normal MODFET. The electrons in the wide bandgap AlGaAs layer are transferred across the heterojunction interface into the smaller bandgap LT-GaAs layer in a manner analogous to the normal MODFET. However, due to the large number of defects present in the LT-GaAs layer, the transferred carriers become trapped and cause the material to have an extremely high resistivity. The transferred charge also gives rise to a negative space charge region on the GaAs side of the heterojunction instead of the two dimensional electron gas (2 DEG) that is normally formed in MODFETs. The presence of the negative space charge in the GaAs and ionized impurities in the AlGaAs doping layer result in pronounced band bending and the creation of a built in electric field perpendicular to the heterojunction plane. This results in the LT-MODFET having a band structure which is very similar in appearance to the band structure of a normal MODFET.

To illustrate this, figure 5.2 shows the band structure in a direction normal to the surface for a normal MODFET and a LT-MODFET in the dark, as obtained from a self-consistent solution of the one dimensional Poisson-Schrödinger equation. From this figure it can be seen that the band structure of the LT-MODFET does appear quite similar to the
Normal MODFET layer structure: 10nm 1E18 Si doped GaAs, 30nm 1E18 Si doped Al0.2Ga0.8As, 15nm undoped Al0.2Ga0.8As, and 500nm undoped GaAs

A) Band Structure of Normal MODFET

LT-MODFET layer structure: 35nm 1E18 Si doped Al0.2Ga0.8As, 15nm undoped Al0.2Ga0.8As, and 500nm undoped LT-GaAs

B) Band Structure of a LT-MODFET

FIGURE 5.2
Simulated conduction band profiles of a normal MODFET and a LT-MODFET.
band structure of the normal MODFET, except that the Fermi level (the Fermi level is referenced to 0 meV for each diagram) is nearly 500meV below the band edge in the LT-MODFET, whereas the Fermi level is close to the conduction band edge for the normal MODFET. The fact that the Fermi level is ~500meV below the conduction band edge in the LT-MODFET indicates that the material has a very low free carrier concentration, and is consistent with the extremely large dark resistivity of the LT-MODFET structure. It can also be seen that both the normal and LT-MODFET have a large built in electric field near the heterointerface resulting in a triangular potential well where quantum confinement of carriers can occur.

The large dark resistivity of the LT-MODFET decreases dramatically when the sample is illuminated. Under illumination, carriers are photogenerated within the LT-GaAs channel region and swept to the heterointerface by the built in field present in the device. At the heterointerface the photogenerated carriers accumulate to form a two dimensional electron gas (2-DEG). The presence of the 2-DEG at the heterointerface moves the Fermi level much closer to the conduction band edge and the LT-MODFET band diagram begins to resemble the band structure of a normal MODFET more closely. Under strong illumination the channel carrier concentrations in the LT-MODFET can attain nearly the same levels found in a normal MODFET; thus the LT-MODFET basically functions like a normally off MODFET that is turned on by light. Due to the similarity of the simulated band structures and device operation of the LT-MODFET and normal MODFET, it is believed that the transport properties of the LT-MODFET under illumination are characteristic of the 2-DEG at the AlGaAs/GaAs heterointerface.
5.4 Experimental Characterization of Material Mobility.

After growth of the LT-MODFET material, the samples were characterized to determine their Hall mobility and resistivity. The Hall test measurement facility used for these measurements consisted of an electromagnet capable of producing up to 8000 Gauss, a specially designed sample holder, and a small Dewar which can be used to cool the sample to liquid nitrogen temperature by immersion into liquid nitrogen. A Keithley model 220 programmable current source, and a model 181 nanovoltmeter interfaced through an IBM compatible PC were used for sample bias and voltage measurement. A specially made switch box was used to connect the current source and voltmeter to the sample contacts in a manner appropriate for making Hall measurements using the van der Pauw method described earlier in section 2.4.

Since the resistivity of the LT-MODFET samples was extremely large unless the samples were illuminated, the sample holder had to be additionally modified to incorporate an optical waveguide to transmit light to the sample during the Hall measurement. This was accomplished using a small square rod of Plexiglas which had a facet on one end which was appropriately angled to reflect light onto the sample surface (see figure 5.3 on the following page). The reflectivity of the light guiding surfaces was increased by evaporating a thin opaque aluminum film onto the Plexiglas. Although this was a relatively simple and crude light guide, it was highly effective in coupling either white light from a tungsten light source or monochromatic laser illumination onto the sample surface. The Plexiglas light guide was also able to withstand immersion into liquid nitrogen without
significant damage. Therefore, this simple setup allowed sample illumination at both 300K and 77K, and enabled Hall measurements to be performed on the LT-MODFET material at both these temperatures.

For the LT-MODFET samples characterized in this study, van der Pauw Hall samples were fabricated subsequent to growth as described below. Since the samples were all grown using indium solder to mount them to the molybdenum growth block, there was a residual coating of indium on the back of the samples subsequent to their removal from the growth block. For samples of low to moderate resistivity grown on semi-insulating GaAs, the indium layer on the back of the sample poses no significant
errors in the Hall measurement due to leakage current traveling through this layer. However, due to the large resistivity of the LT-MODFET material used in this study, the indium on the back of the samples could cause an error in the Hall measurement, and had to be removed prior to fabrication of van der Pauw Hall samples. This was accomplished by mounting the sample to a polishing jig and lapping the indium from the sample back in a silicon carbide slurry. Once the indium had been removed from the sample back, the sample was cleaved into ~5mm x 5mm squares and ohmic contacts were then made to the samples in the Van der Pauw Hall geometry discussed in section 2.4. In(90%)/Sn(10%) contacts were alloyed to four points on the sample in an annealing furnace at 450°C in a forming gas ambient for 4 minutes and then checked to insure that the ohmic contacts were adequate to allow Hall measurements to be made.

### 5.5 Mobility Measurement Results

The results of the Van-der-Pauw Hall mobility measurements are summarized in table 5.1 below. The measured mobilities of the 2-DEG in these samples are in the range of 500 to 750 cm²/V·s at 300K and ~3000 to 5000 cm²/V·s at 77K. The room temperature mobility of these samples is in the same range as the Hall mobilities of single layers of LT-GaAs reported in the literature [54]. The mobility of LT-GaAs at 77K had never been reported prior to this study, and was first published in reference [60]. Since the Hall mobilities can be measured even at temperatures as low as 77K, it appears that band conduction is dominant in LT-GaAs MODFET samples under illumination. From the
results in table 5.1 it can also be seen that the inclusion of a 65Å spacer layer of GaAs grown at 580°C between the LT-GaAs and the AlGaAs modulation doping layers has only a small effect since the mobilities measured in the samples including a spacer layer show only a small increase over the samples which have no spacer.

Since the mobility of normal MODFET structures exhibits a dependence upon the channel carrier concentration, it seems reasonable to expect similar behavior from LT-MODFET material. During the measurement of the LT-MODFET sample mobilities, it was observed that the mobilities did indeed exhibit a dependence upon channel carrier concentration. In order to investigate this effect more fully, the concentration dependence of one of the samples was measured and is shown in figure 5.4. In order to vary the channel carrier density, the intensity of light used to illuminate the sample was varied. Unfortunately, at room temperature it was not possible to determine the dependence of mobility upon the carrier concentration since the light source used in our system was unable to create a significant change in carrier concentration at this temperature. However, at 77K the light source created sufficient changes in carrier concentration to

<table>
<thead>
<tr>
<th>Sample #</th>
<th>Growth Temperature (°C)</th>
<th>Spacer Thickness (Å)</th>
<th>300K Mobility (cm²/V·s)</th>
<th>77K Mobility (cm²/V·s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-22-12-93</td>
<td>250</td>
<td>0</td>
<td>650</td>
<td>3600</td>
</tr>
<tr>
<td>1-13-1-94</td>
<td>250</td>
<td>65</td>
<td>770</td>
<td>4880</td>
</tr>
<tr>
<td>1-13-12-93</td>
<td>300</td>
<td>0</td>
<td>500</td>
<td>---</td>
</tr>
<tr>
<td>1-3-1-94</td>
<td>300</td>
<td>65</td>
<td>550</td>
<td>5500</td>
</tr>
<tr>
<td>2-20-12-93</td>
<td>350</td>
<td>0</td>
<td>750</td>
<td>5500</td>
</tr>
</tbody>
</table>
allow a reasonable measurement of mobility versus channel carrier density. In figure 5.4 it can be clearly seen that the mobility in these samples is highly dependent upon the sheet carrier concentration.

In the light of this strong dependence of the mobility upon sheet carrier density, a few additional comments about the data presented in table 5.1 should be mentioned. Every effort was made to insure that the intensity of the light used for sample illumination was the same for each measurement presented in this table. Also, the illumination used to determine the mobilities presented in this table was essentially at the maximum level attainable from the light source available in our system. It is therefore believed that the variations in mobility observed in table 5.1 are most likely due to other factors besides channel carrier density differences, and that the mobilities presented in the table should be considered as upper limits on the mobility in these samples. Since the arsenic cluster size

![FIGURE 5.4](image)

**FIGURE 5.4**

Mobility versus channel carrier density for sample #1-3-1-94.
and density of clusters are both highly dependent on the sample growth temperature and post sample annealing, and these parameters have a large effect upon mobility in LT-GaAs material, it seems more likely that the variations in mobilities from sample to sample are due to differences in the size and density of arsenic clusters present in the samples.

5.6 Simulation of Mobility

In order to understand more fully the mobility measurements in the LT-MODFET structures we have calculated the low field mobility in these structures based on a simple scattering model. The computer program used numerical integration to solve the Boltzmann Transport Equation in the relaxation time approximation. The distribution function \( f(\vec{r},\vec{p},t) \) gives the probability that a carrier with crystal momentum \( \vec{p} \) will be found at position \( \vec{r} \) at time \( t \). The Boltzmann equation given below, essentially describes the change in the one particle distribution function, \( f(\vec{r},\vec{p},t) \), by accounting for all possible mechanisms which may alter \( f(\vec{r},\vec{p},t) \). In this equation, the collision term, 

\[
\frac{\partial f(\vec{r},\vec{p},t)}{\partial t} + \nu \cdot \nabla f(\vec{r},\vec{p},t) + F \cdot \nabla_p f(\vec{r},\vec{p},t) = s(\vec{r},\vec{p},t) + \frac{\partial f(\vec{r},\vec{p},t)}{\partial t} \]

the change in the one particle distribution function, \( f(\vec{r},\vec{p},t) \), by accounting for all possible mechanisms which may alter \( f(\vec{r},\vec{p},t) \). In this equation, the collision term, 

\[
\left. \frac{\partial f(\vec{r},\vec{p},t)}{\partial t} \right|_{\text{coll}},
\]

describes the change in the distribution function due to scattering processes. It is therefore the solution to the collision integral which is the main concern in calculating the carrier mobility. In the relaxation time approximation, scattering events are assumed
to be elastic, and for the purposes of this work only low applied fields are considered. Under these assumptions, the collision term can be written as: [61]

\[ \frac{\partial f(\vec{r},\vec{p},t)}{\partial t} \bigg|_{\text{coll}} = -\frac{f_\Lambda(\vec{r},\vec{p},t)}{\tau_\ell} = \frac{f(\vec{r},\vec{p},t) - f_0(\vec{r},\vec{p},t)}{\tau_\ell}, \]

where \( f_0(\vec{r},\vec{p},t) \) is the equilibrium distribution function and \( \tau_\ell \) is a characteristic time which describes how the distribution function relaxes. The time \( \tau_\ell \) (usually called \( \tau_m \) or \( \tau_{el} \)) can be calculated from the following equation:

\[ \frac{1}{\tau_{el}} = \int d\vec{k} (1 - \cos \theta_k) S_{el}(\vec{k},\vec{k}') \]

The relaxation times for several different scattering mechanisms can be combined to calculate a total relaxation time in the following manner:

\[ S_{el}(E) = \frac{1}{\tau_{\text{Total}}(E)} = \frac{1}{\tau_1(E)} + \frac{1}{\tau_2(E)} + \frac{1}{\tau_3(E)} + \cdots + \frac{1}{\tau_n(E)} \]

Once the relaxation time for the combined scattering mechanisms for a given energy has been calculated in this manner, the mobility, \( \mu \), is be determined by averaging the total relaxation time over the electron energy distribution using the following equation:

\[ \mu = \frac{e \langle \tau_{\text{Total}} \rangle}{m^*} \quad \text{where} \quad \langle \tau \rangle = \frac{\int_{E_0}^{\infty} \tau(E) E \left( \frac{\partial f_0}{\partial E} \right) dE}{\int_{E_0}^{\infty} E \left( \frac{\partial f_0}{\partial E} \right) dE} \quad \text{and} \quad f_0 = \frac{1}{1 + e^{(E-E_f)/kT}} \]

A more detailed derivation of these equations and more thorough discussion of the solution of the Boltzmann equation can be found in reference [62].

A relaxation time, \( \tau_n \), as defined above, can be obtained for all the elastic scattering processes. However, for scattering events which are inelastic in nature, such as polar optic
phonon scattering, a simple relaxation time as defined above can not generally be
determined. If both inelastic and elastic scattering processes are included in the collision
term, the Boltzmann equation can be cast in the following form: [62]

\[ 1 = \left[ S_a(E) + S_o(E) \right] \phi(E) - S_a(E) \phi(E + \hbar \omega_q) - S_o(E) \phi(E - \hbar \omega_q) \]

where \( \phi(x) \) is a step function such that \( \phi(x) = 1 \) for \( x > 0 \) and \( \phi(x) = 0 \) for \( x \leq 0 \), \( S_a(E) \) corresponds to the rate at which electrons are scattered out of the state \( \vec{k} \), and \( S_o(E) \) and
\( S_o(E) \) correspond to the rate at which electrons are scattered into the state \( \vec{k} \) due to the
absorption and emission of phonons of energy \( \hbar \omega_q \). \( S_o(E) \) denotes the sum of the
relaxation times of the electrons for elastic scattering mechanisms. For this work, only the
scattering by polar optical phonons is treated as an inelastic process.

In general, when both elastic and inelastic scattering processes are present, a
numeric iterative method, such as the technique of Rode [63], must be used to solve the
Boltzmann equation and calculate the carrier mobility. However, for calculations at
temperatures below \( \sim 77K \), a simpler non-iterative approach can be used without incurring
significant errors due to the inelastic nature of the polar optic phonon scattering process.
For this work, the measurements being simulated were all performed at 77K, and therefore
the simpler non-iterative approach was used. Also, for computational simplicity, the in-
scattering for polar optic phonons was neglected in this work. This will cause the
scattering rate for polar optical phonon scattering to be somewhat overestimated. Even
though these computational simplifications increase the effect of polar optic scattering on
the mobility, the results of the simulation show that the scattering due to polar optical
phonons plays an insignificant role in determining the overall carrier mobility in the LT-
MODFET, and thus the errors introduced into the final mobility values by using these simplifications are minimal. These calculations were intended to provide a first order approximation to determine the effect that arsenic clusters have upon carrier mobility in the LT-GaAs MODFET channel, and should serve as a basis for further, more complete analysis.

The importance of understanding normal MODFET technology has led to the derivation of expressions for the scattering rate of electrons in such quasi two-dimensional systems by several groups. [62,64,65] Due to the two dimensional confinement present in the LT-MODFET and its similarity to normal MODFET structures, this work was based upon these scattering rates; however, a new scattering mechanism was added to account for the presence of arsenic clusters in the LT-GaAs channel in the LT-MODFET.

In order to cast the scattering rates in a closed analytical form, the standard variational form of the ground state wavefunction of the 2-DEG as derived by Fang and Howard [66] was used. This wave form assumes that the ground state wavefunction $\chi(z)$ is given by the following:

$$\chi(z) = \left( \frac{\hbar^3}{2} \right)^{1/2} e^{-b z/2}$$

where $b$ is chosen to minimize the ground state energy $\langle E \rangle$ given by:

$$\langle E \rangle = \langle \chi_0 | E | \chi_0 \rangle = \langle \chi_0 | -\frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + V(Z) \chi_0 \rangle$$

When $\langle E \rangle$ is minimized with respect to the variational parameter $b$, it can be shown that the variational parameter $b$ is given by:
\[ b = \left( \frac{12q^2m_z}{\hbar^2\varepsilon_0\varepsilon_r} \left( N_{\text{dop}} + \frac{11}{32} N_s \right) \right)^{1/3} \]

and the average width of the inversion layer charge is given by \( Z_{\text{avg}} \approx \frac{3}{b} \).

Using the variational form of the wavefunction shown above, closed form expressions for the scattering matrix elements and relaxation times can be obtained. For this work the following scattering mechanisms have been included: (i) scattering by polar optical phonons (ii) scattering by acoustic phonons through the deformation potential coupling and piezoelectric coupling (iii) scattering by ionized impurities in the doped AlGaAs, spacer AlGaAs and in the channel LT-GaAs regions and (iv) scattering by arsenic clusters, assuming the clusters to be hard spheres of potential \( \phi_{\text{bn}} \). Since the closed analytical form of the relaxation times for the first three mechanisms have been widely used and referenced in the pertinent literature, only the analytic expressions for the relaxation times will be presented here. The reader is referred to references [62],[64] and [65] for a more detailed derivation of these expressions. The rate for scattering due to the arsenic clusters will be derived fully since this is the first time such a scattering mechanism has been employed in a two dimensional mobility calculation.

The scattering rate of carriers out of the state \( \vec{k} \) due to interaction with polar optical phonons can be expressed by the following equation:

\[
S_0(E) = B \left[ (N_q + 1) \left[ 1 - f_0 \left( E - \hbar \omega_q \right) \right] H_1(Y_-) + N_q \left[ 1 - f_0 \left( E + \hbar \omega_q \right) \right] H_1(Y_+) \right] \]

(1)

where \( B, H_1(Y_-) \) and \( H_1(Y_+) \) are given by the following expressions:
\[ B = \frac{e^2 \hbar \omega_q}{64 \pi \varepsilon_0} \left( \frac{1}{\kappa_{\omega}} + \frac{1}{\kappa_S} \right) \frac{m^*}{\sqrt{2 E \hbar^2 \left[ 1 - f_0(E) \right]}} \]

\[ H_1(Y_\pm) = \frac{2\pi}{\sqrt{1 + X_\pm - 2 \sqrt{X_\pm \cos \theta}} (Y_\pm + b)^3} \]

\[ X_\pm = \frac{(E \pm \hbar \omega_q)}{E} \quad Y_\pm = \left( \frac{2m^* E}{\hbar} \right)^{1/2} \left[ 1 + X_\pm - 2 \sqrt{X_\pm \cos \theta} \right]^{1/2} \]

Similar rates, \( S_a(E) \) and \( S_e(E) \), corresponding to scattering into the state \( \vec{k} \) due to the absorption and emission of phonons of energy \( \hbar \omega_q \), can also be defined. Although the in-scattering events described by \( S_a(E) \) and \( S_e(E) \) have been neglected in this simulation as mentioned above, their rates have been included here in equations 2 and 3 to follow, for the sake of completeness.

\[ S_a(E) = B N_q \left[ 1 - f_0(E + \hbar \omega_q) \right] \sqrt{X_+} H_2(Y_+) \quad (2) \]
\[ S_e(E) = B \left( N_q + 1 \right) \left[ 1 - f_0(E - \hbar \omega_q) \right] \sqrt{X_-} H_2(Y_-) \quad (3) \]

where \( H_2(Y_\pm) = \frac{2\pi}{\sqrt{1 + X_\pm - 2 \sqrt{X_\pm \cos \theta}} (Y_\pm + b)^3} \cos \theta d\theta \) and \( B, X_\pm, \text{and } Y_\pm \) are defined the same as in \( S_0(E) \).

The relaxation time for scattering by acoustic phonons through the deformation potential is given by the following equation:

\[ \frac{1}{\tau_{ac}} = \frac{\left( 3bD^2 m^* k_b T e^2 \right)}{16 \hbar^5 C_i} \quad (4) \]

Where \( D \) is the acoustic deformation potential and \( C_i = \frac{1}{3} \left( 3C_{11} + 2C_{12} + 4C_{44} \right) \) is the longitudinal elastic constant.
The relaxation time for scattering by acoustic phonons coupled through piezoelectric interaction is given by:

\[
\frac{1}{\tau_{pz}} = \frac{e^2 m^* K^2 k_b T b^2 \pi}{32 \pi \hbar \varepsilon_0 \varepsilon_r} \int_0^{2\pi} \frac{(8b^3 + 9bq^3 + 3q^2)}{8q(q + b)^3} (1 - \cos \theta) \, d\theta
\]  

(5)

where \( q = 2k \sin \left( \frac{\theta}{2} \right) = 2 \sqrt{\frac{2m^* E}{\hbar^2}} \sin \left( \frac{\theta}{2} \right) \) is the parallel component of the scattered wave vector and \( K \) is the dimensionless piezoelectric constant.

Finally, the relaxation time for scattering by ionized impurities can be broken into two separate parts, the first part due to the ionized impurities in the GaAs channel region and the second part due to the ionized impurities in the AlGaAs layers (including both the doped AlGaAs layer and the spacer AlGaAs layer). The relaxation time for scattering by the ionized impurities in the GaAs channel is given by the following equation:

\[
\frac{1}{\tau_{ii}} = \frac{e^4 m^*}{8\pi \hbar^3 \varepsilon_0^2 \varepsilon_r^2} \int_0^{2\pi} \frac{N_B C_0 (1 - \cos \theta) \, d\theta}{2q(q + q_s F(q))^2}
\]  

(6)

where \( N_B \) is the impurity concentration, \( F(q) = \frac{(8b^3 + 9b^2 + 3bq^2)}{8(b + q)^3} \) is the form factor, \( q_s \) is the screening parameter and

\[
q_s = \frac{2\pi e^2 N_s}{\varepsilon_0 \varepsilon_r k_b T} \left[ \left( 1 + e^{-E_F/k_b T} \right) \ln \left( 1 + e^{E_F/k_b T} \right) \right]
\]

\[
C_0 = \frac{(2b^5 + 24b^5q + 48b^4q^2 + 43b^3q^3 + 18b^2q^4 + 3bq^5)}{2(b + q)^6}
\]
The relaxation time for scattering by the remaining ionized impurities in the AlGaAs layers, (usually referred to as remote impurity scattering since these impurities are spatially separated from the carriers confined in the GaAs channel) is given by equation 7:

\[
\frac{1}{\tau} = \frac{e^4 m^*}{8\pi h^3 e_o^2 \varepsilon_r^2} \left[ \frac{2\pi N_D}{\int_0 ^{2\pi} \frac{P_0^2 \left( e^{-2q_{ts}} - e^{-2q_{tp}} \right)}{2q(q + q_s F(q))^2} (1 - \cos\theta) d\theta + \frac{2\pi N_{sp}^2}{\int_0 ^{2\pi} \frac{P_0^2 \left( 1 - e^{-2q_{ts}} \right)}{2q(q + q_s F(q))^2} (1 - \cos\theta) d\theta} \right]
\]

where \( N_D \) is the impurity concentration in the doped region, \( N_{sp} \) is the impurity concentration in the spacer region, \( t_s \) is the thickness of the spacer layer, \( t_D \) is the total thickness of the spacer and doping layers, \( P_0 = b^3/(b + q)^3 \), and \( q_s \) and \( F(q) \) are defined the same as in equation 6.

The scattering mechanisms discussed above, polar optical phonon scattering, acoustic and piezoelectric phonon scattering, and ionized and remote impurity scattering, account for the most common and important scattering events in a normal MODFET structure. In the new LT-MODFET structure; however, arsenic clusters are formed by precipitation of the excess arsenic present in the LT-GaAs channel during the growth of the AlGaAs layers. In order to account for the presence of these clusters and their effect upon the mobility of carriers in the LT-MODFET, a new scattering mechanism was added in this study. This new scattering mechanism, which will be referred to as cluster scattering, is based upon a modified alloy disorder scattering normally present in InGaAs channel MODFETs.
Given any scattering potential, the procedure for calculating a scattering rate is essentially the same for all scattering mechanisms. The basis for such calculations is a quantum mechanical statement of the rate of transfer of carriers from state $\vec{k}$ to state $\vec{k}'$ and energy conservation commonly known as Fermi’s Golden Rule. Mathematically this is given as:

$$\Gamma_{\vec{k},\vec{k}'} = \frac{2\pi}{\hbar} |H_{\vec{s}}^{\vec{k},\vec{k}'}|^2 \delta(E_{\vec{k}'} - E_{\vec{k}} \pm \hbar \omega_q) \tag{8}$$

where $\Gamma_{\vec{k},\vec{k}'}$ is the rate of scattering state $\vec{k}$ to state $\vec{k}'$ which depends upon a matrix element $|H_{\vec{s}}^{\vec{k},\vec{k}'}|^2$ describing the strength of scattering. The delta function insures that scattering events conserve energy, and $E_{\vec{k}'}$ equals $E_{\vec{k}}$ plus or minus a quantum of phonon energy $\hbar \omega_q$ which can be absorbed or lost in the scattering event.

In order to use Fermi’s Golden Rule, one must first calculate the scattering matrix element $|H_{\vec{s}}^{\vec{k},\vec{k}'}|^2$. The scattering matrix element depends on the scattering potential $V_s(\vec{r})$, which represents a small perturbation in the crystal potential caused by a phonon or impurity. Given the scattering potential $V_s(\vec{r})$, the scattering matrix element can be calculated from equation 9.

$$|H_{\vec{s}}^{\vec{k},\vec{k}'}|^2 = \left| \left(\Psi_{\vec{k}'}^* \right| V_s(\vec{r}) \left| \Psi_{\vec{k}} \right) \right|^2 = \int d\vec{r} \Psi_{\vec{k}'}^* (\vec{r}) V_s(\vec{r}) \Psi_{\vec{k}} (\vec{r})^2 \tag{9}$$

For the case of a two dimensional system such as a MODFET, the integral in equation 9 can be evaluated most easily in cylindrical coordinates, where the integral can be further broken down into two parts, one describing the interaction of the wavefunction of the 2-DEG and the scattering center, and the other part describing the interaction of the carriers
and the scattering center in the unconfined directions. The quantum confinement in a MODFET device is in the direction perpendicular to the heterointerface, and this direction is typically labeled as the z direction, and the wavefunction describing the carrier distribution in this direction as \( \chi(z) \). The directions perpendicular to the z direction, in which the carriers are not quantum confined, characterized by the coordinates \( r \) and \( \theta \).

Using these coordinates, the integral in equation 9 can be written as follows:

\[
\left| H_{s_{\bar{k},\bar{k}'}} \right|^2 = \left| \frac{1}{V} \int d\bar{r} \Psi_{k_{\bar{k}}}^*(\bar{r}) V(\bar{r}) \Psi_{k_{\bar{k}'}}(\bar{r}) \right|^2 = \left| \frac{1}{V} \int |\chi_{0}(z)|^2 dz \int_0^{\infty} r dr \ e^{-i\bar{q} \cdot r} V(r,\theta) e^{i\bar{k} \cdot r} \right|^2
\]

\[
\left| H_{s_{\bar{k},\bar{k}'}} \right|^2 = \frac{1}{V^2} \left| \int |\chi_{0}(z)|^2 dz \int_0^{\infty} r dr \ e^{-i\bar{q} \cdot r} V(r,\theta) \right|^2
\]

\[
\left| H_{s_{\bar{k},\bar{k}'}} \right|^2 = \frac{1}{V^2} \left| \int |\chi_{0}(z)|^2 dz \int_0^{\infty} r dr J_0(q \cdot r) V(r) \right|^2, \quad (10)
\]

where \( \bar{q} = \bar{k}' - \bar{k} \) is the scattering vector, \( J_0 \) is the zero order Bessel function, \( \chi_{0}(z) \) is the variational wavefunction given on page 72, and \( V(r,\theta) \) has been assumed to be radially symmetric and depend only upon \( r \). Once the scattering matrix element has been determined, and the scattering rate from Fermi’s Golden Rule has been obtained, assuming the scattering is elastic (i.e. no energy is lost in the scattering event) and only low fields are present, a two dimensional energy relaxation time \( \frac{1}{\tau} \) can be defined from \( \Gamma_{\bar{k},\bar{k}'} \), and is given by the following:

\[
\frac{1}{\tau} = \frac{V}{(2\pi)^2} \int \Gamma_{\bar{k},\bar{k}'} (1 - \cos\theta) \bar{k}' \, d\bar{k}' \, d\theta \quad (11)
\]

In order to simplify the evaluation of this integral, the integration over \( \bar{k}' \) can be converted to an integral over energy. Since no energy is lost as a result of an elastic
scattering event, \( k' = k \) and the scattering vector \( \mathbf{q} = \mathbf{k}' - \mathbf{k} \) can be written as

\[
q^2 = |\mathbf{k}' - \mathbf{k}|^2 = k'{}^2 + k^2 - 2 k' k \cos \theta = 2 k^2 - 2 k^2 \cos \theta = 2k^2 (1 - \cos \theta) = 2k^2 \sin^2 \frac{\theta}{2}
\]

and thus \( q = 2k \sin \frac{\theta}{2} = 2 \sqrt{\frac{2m^* E}{\hbar^2}} \sin \frac{\theta}{2} \). Also, since \( k^2 = \frac{2m^* E}{\hbar^2} \), \( 2kdk = \frac{2m^* dE}{\hbar^2} \), thus \( kdk = \frac{m^* dE}{\hbar^2} \). Substituting these into equation 11, the energy relaxation time is given by:

\[
\frac{1}{\tau} = \frac{V}{(2\pi)^2} \int \Gamma_{k,k'}^k \left(1 - \cos \theta\right) \frac{m^*}{\hbar^2} dE d\theta \quad (12)
\]

Although the scattering vector \( q \) does not appear explicitly in equation 12, it will always be present due to the bessel function \( J_0(qr) \) found in the matrix element \( |H_{ks,k'}^k|^2 \) given in equation 10. Therefore the conversion of \( q \) to energy given above will be needed to accomplish the actual integration given in equation 12.

Thus with equations 8, 10, and 12, and a knowledge of the scattering potential \( V(z,r,\theta) \) which describes the way carriers are scattered by a particular defect, a relaxation time can be calculated for any elastic scattering mechanism. Assuming scattering from arsenic clusters to be elastic, the remaining tasks to determine a relaxation time for cluster scattering are to determine a scattering potential \( V(r) \) which describes the arsenic clusters, and to evaluate the integral describing the interaction of the variational wavefunction \( \chi(z) \) with the clusters.

To evaluate the integral over \( \chi(z) \) given in equation 10, the clusters are assumed to be cylinders of radius \( r_0 \) centered at \( z_0 \). Then the interaction of a single cluster and the
variational wavefunction can be defined as \( \phi(z_i) \), where \( \phi(z_i) = \int_{z_i-r_0}^{z_i+r_0} |\chi(z)|^2 \, dz \) and thus,

\[
|\phi(z_i)|^2 = \int_{z_i-r_0}^{z_i+r_0} |\chi(z)|^2 \, dz .
\]

However, since \( |\phi(z_i)|^2 \) only accounts for the interaction of \( \chi(z) \) and a single cluster, this term must be summed over all the cluster sites in order to account properly for the scattering due to all the clusters present in the device. Thus, when \( |\phi(z_i)|^2 \) is summed over all the cluster sites, the integral of \( |\chi(z)|^2 \, dz \) in equation 10 can be replaced by this sum and equation 10 can be rewritten as follows:

\[
\left| H_{s,k'} \right|^2 = \frac{1}{V^2} \sum_{N_xN_z} |\phi(z_i)|^2 \left| 2\pi \int_0^\infty r dr J_0(\bar{q}r) V(r,\theta) \right|^2
\]

where \( N_x \) and \( N_z \) denote, respectively, the number of cluster sites over the surface and along the z direction. If \( N_{ci} \) is the volume density of arsenic clusters present in the channel region, this sum can be converted to an integral and simplified further to give equation 14.

\[
\sum_{N_xN_z} |\phi(z_i)|^2 = \frac{V}{b N_x N_z} \int_{-b}^{b} dz_i |\phi(z_i)|^2 = \frac{V}{b N_{ci} F(z_i)}
\]

where \( F(z_i) = \frac{1}{4 \bar{a}} \int_{-b}^{b} \left( e^{-\bar{a} y_1} (y_1^2 + 2y_1 + 2) - e^{-\bar{a} y_1} (y_2^2 + 2y_2 + 2) \right) dy \), \( y_2 = y_1 + 2r_0, y_1 = y - br_0 \), and \( w \) is the width of the LT-GaAs layer. Now substituting equation 14 into equation 13, the matrix element \( |H_{s,k'}|^2 \) can be written:

\[
|H_{s,k'}|^2 = \frac{1}{Vb} N_{ci} F(z_i) \left| 2\pi \int_0^\infty r dr J_0(\bar{q}r) V(r,\theta) \right|^2
\]

From equation 15 it only remains to specify the scattering potential \( V(r) \) and perform the integration over \( r \) to calculate the scattering matrix element. As a first approximation, the
arsenic clusters were considered to be hard spheres of radius \( r_0 \) with a potential barrier height of \( \phi_{bn} \), where \( \phi_{bn} \) is the Schottky barrier height of arsenic on GaAs. This potential is shown schematically in figure 5.5a on page 82. Essentially this scattering potential is a radially symmetric square potential barrier and models the arsenic cluster as a solid sphere, where scattering events can best be described as billiard ball like collisions with the arsenic cluster. Placing this potential into equation 15, and integrating over \( r \), the following closed form can be obtained for the scattering matrix element:

\[
\left| H^{k',k} \right|^2 = \frac{1}{V \beta} N_{cl}(z_i) \left| 2\pi \int_0^r dr J_0(\bar{q}r) \phi_{bn} \right|^2 = \frac{4 \pi^2 \phi_{bn}^2 r_0^2}{V \beta} N_{cl}(z_i) \left| \frac{J_1(\bar{q}r_0)}{\bar{q}} \right|^2
\]

where \( J_1 \) is the bessel function of order 1. Now inserting equation 16 into equation 8, the scattering rate \( \Gamma_{k,k'} \) can be expressed as follows:

\[
\Gamma_{k,k'} = \frac{2\pi}{\hbar} \left| H^{k,k'} \right|^2 \delta(E_{k'} - E_k) = \frac{8\pi^3 \phi_{bn}^2 r_0^2}{\hbar V b q^2} N_{cl}(z_i) \left| J_1(\bar{q}r_0) \right|^2 \delta(E_{k'} - E_k)
\]

Using the scattering rate calculated in equation 17 it is now possible to compute the relaxation time for scattering due to arsenic clusters using equation 12. Substituting equation 17 into equation 12, the relaxation time for arsenic cluster scattering due to a radially symmetric square potential barrier is given by equation 18 below:

\[
\frac{1}{\tau_{cl}} = \frac{V}{(2\pi)^2} \int_0^{2\pi} \int_0^{\infty} \frac{8\pi^3 \phi_{bn}^2 r_0^2}{\hbar V b q^2} N_{cl}(z_i) \left| J_1(\bar{q}r_0) \right|^2 \delta(E_{k'} - E_k)(1 - \cos\theta) \frac{m^*}{\hbar^2} dE d\theta
\]

\[
= \frac{2\pi \phi_{bn}^2 r_0^2}{\hbar b} N_{cl}(z_i) \int_0^{2\pi} \int_0^{\infty} \frac{J_1(\bar{q}r_0)}{2k^2(1 - \cos\theta)} \delta(E_{k'} - E_k)(1 - \cos\theta) \frac{m^*}{\hbar^2} dE d\theta
\]

\[
= \frac{2\pi \phi_{bn}^2 r_0^2}{\hbar b} N_{cl}(z_i) \int_0^{2\pi} \int_0^{\infty} \frac{J_1(\bar{q}r_0)}{4E} \delta(E_{k'} - E_k) dE d\theta
\]

\[
\frac{1}{\tau_{cl}} = \frac{\pi \phi_{bn}^2 r_0^2}{2\hbar b E} N_{cl}(z_i) \int_0^{2\pi} \left| J_1(\bar{q}r_0) \right|^2 d\theta
\]
FIGURE 5.5
Schematic representation of arsenic cluster and possible scattering potentials. a) square potential barrier, b) Schottky barrier potential, c) combined Schottky and square potential.
The relaxation time in equation 18 gives a reasonable first approximation to the effect arsenic clusters have upon the carrier mobility in the LT-MODFET. However, the use of a spherically symmetric square potential barrier for the scattering potential is most likely an inaccurate representation. The most accepted theory describing the high resistivity of LT-GaAs assumes that the arsenic clusters can be modeled as semi-metallic spheres which will behave like Schottky barriers. This theory attributes the large resistivity of LT-GaAs to the overlap of the Schottky barrier depletion regions surrounding the arsenic clusters, which causes the material to be totally depleted of carriers. Assuming that the Schottky barrier model is an accurate description of the effect of an arsenic cluster in LT-GaAs, it seems that it would be more correct to use a simple Schottky barrier potential to describe the scattering from these clusters. In order to investigate the effect of a Schottky barrier potential upon the mobility, the original program was modified to incorporate a relaxation time calculated using a scattering potential \( V(r) \) in equation 10 which modeled the Schottky potential more accurately than the spherically symmetric square potential barrier used to derive equation 18. A simple Schottky barrier potential is shown schematically in figure 5.5b on page 82, and can be represented mathematically by the following equation:

\[
V(r) = \phi(r) = \frac{qN_D}{\varepsilon_r \varepsilon_0} \left[ \frac{(r-r_0)^2}{2} - (r-r_0)W_d \right] + \phi_{bn} \quad \text{where} \quad W_d = \sqrt{\frac{2\varepsilon_0 \varepsilon_r V_{bi} - e^{-kT/q}}{qN_D}}
\]

In this equation \( W_d \) is the depletion width associated with the Schottky barrier and \( r_0 \) is the radius of the arsenic cluster.
In describing the scattering due to the arsenic clusters, this potential is still not quite adequate, due to the fact that this potential will allow scattering of carriers even when \( r \leq r_0 \), and the only carriers which may be found in the range \( 0 \leq r \leq r_0 \) are carriers trapped within the arsenic cluster itself, and will not generally contribute to the current flow in the LT-GaAs layer. Also since the program is only intended as a simple first order model, there is no mechanism included in the program which could account for trapping of carriers by the arsenic cluster and emission of carriers from a cluster. Since trapping and emission of carriers from an arsenic cluster will attain an equilibrium rate under steady state conditions, and thus not alter the net carrier concentration, it seems reasonable to use a combined potential such as that shown in figure 5.5c, which models the clusters as "soft" spheres and does not allow the presence of carriers in the region \( 0 \leq r \leq r_0 \).

Mathematically this potential is given by equation 19.

\[
V(r) = \phi_{bn} \quad 0 \leq r < r_0 \quad \text{and} \quad V(r) = \phi(r) = \frac{qN_D}{\epsilon_0 \epsilon_r} \left[ \frac{(r - r_0)^2}{2} - \frac{(r - r_0)W_d}{r_0} \right] + \phi_{bn} \quad r_0 \leq r \leq r_0 + W_d \tag{19}
\]

Unfortunately, when this potential is used, a simple form for the relaxation time involving only an integration over \( \theta \) is not easily obtainable, and the integration over \( r \) must also be done by numerical methods. If one follows the procedure outlined to arrive at equation 18 using an arbitrary potential \( V(r) \), the simplest form of the relaxation time attainable is:

\[
\frac{1}{\tau} = \frac{2\pi n^* e^2 N_{cl}}{\hbar^3} \cdot F(z_i) \int_0^{2\pi} \frac{(1 - \cos \theta)}{2q(q + q,F(q))} \left| J_0(qr) V(r) rdr \right|^2 d\theta \tag{20}
\]

Equation 20 is valid for any radially symmetric potential \( V(r) \) and usually the infinite upper limit on the integration over \( r \) will not present a problem, since the extent of most real
scattering potentials is limited to a small region and therefore this limit will usually be much less than \( \infty \). In the case of the scattering potential given on the previous page, the integration will be from 0 to \( r_0 + W_d \) and is therefore easily integrated using a variety of available numerical methods.

The particular numerical method chosen to perform the integrations in this program was a simple sixteen point Gaussian Quadrature routine. In order to increase accuracy in integration and prevent errors due to large integration intervals, a subroutine was created to break up an integration into a user definable number of smaller regions, each of which could be integrated accurately using the Gaussian Quadrature method. This subroutine allows the user to optimize each integration for both speed and numerical accuracy by simply specifying the number of subintervals necessary to correctly evaluate a particular integral.

5.7 Computer Simulation Results and Comparison With Experimental Data

The computer program outlined earlier was originally implemented with the relaxation time for arsenic cluster scattering given by equation 18. This equation was arrived at by assuming that the scattering potential of the arsenic clusters could be modeled as a constant potential \( V(r) = \phi_{ba} \) for \( 0 \leq r \leq r_0 \) and \( V(r) = 0 \) elsewhere, where \( \phi_{ba} \) is the Schottky barrier height in GaAs. Using this program, the mobility could be calculated as either a function of temperature or channel carrier density. Since the facilities available at the time of the experiments did not allow easy measurement of the
temperature dependence of mobility in these samples, it was decided to use the program to attempt to model the mobility versus channel carrier density data obtained in figure 5.5.

In order to check the accuracy of the program, the calculated dependence of mobility limited by each scattering mechanism, and the total mobility, upon the channel carrier density at 77 K are plotted in figure 5.6. The parameters used in this calculation are typical for the LT-MODFET structures used in this study (see parameters used for calculation of figure 5.7). The mobility versus carrier density curves calculated for each

![Graph showing mobility versus carrier density for various scattering mechanisms.](image)

**FIGURE 5.6**

Calculated mobility versus carrier concentration for various scattering mechanisms.
scattering mechanism, with the exception of polar optical phonon and arsenic cluster scattering, were all found to be in good agreement with published results. As was mentioned in the discussion of the simulation program, the in scattering events were neglected for the polar optical phonon scattering and this yields a lower mobility than would normally be expected for this mechanism. In spite of this, it can be seen from figure 5.6 that the scattering due to polar optical phonons does not play a significant role in limiting the mobility in these structures. From this figure is evident that the mobility in the LT-MODFET model is mainly limited by the arsenic cluster scattering and the ionized impurity scattering in the LT-GaAs channel region.

Once the accuracy of the program had been checked, the program was run several times systematically varying the cluster radius, density of clusters and density of ionized impurities in the LT-GaAs channel region in order to find a best fit to the data in figure 5.5. The results of this are shown in figure 5.7 where the parameters used to obtain the fit.

![Figure 5.7](image_url)

**FIGURE 5.7**
Comparison of calculated and measured mobility versus channel carrier concentration.
are as follows: cluster concentration \( (N_{cl}) = 10^{16} \text{ cm}^{-3} \), cluster diameter \( 2r_0 = 50\text{Å} \), ionized impurity concentration in the channel \( (N_i) = 10^{18} \text{ cm}^{-3} \), concentration of background impurities in the undoped AlGaAs layer \( (N_B) = 10^{15} \text{ cm}^{-3} \), doping concentration in the doped AlGaAs region \( (N_D) = 10^{18} \text{ cm}^{-3} \), thickness of the undoped AlGaAs \( (t_s) = 150\text{Å} \), and thickness of the doped AlGaAs layer \( (t_d) = 350\text{Å} \). From figure 10 it can be seen that these parameters give a reasonably good first order fit to the data. The Cluster diameter and concentration of the clusters are in the same range as those reported for typical short-time annealed LT-GaAs samples from TEM observation [67]. The ionized impurity concentration in the channel is also in reasonable agreement with the trap concentration in annealed LT-GaAs reported from other groups [68].

Although this calculation gave a reasonable first order fit to the data, clearly the simulation needed to be improved to model the scattering by arsenic clusters more accurately. In order to accomplish this a second version of the program was coded which modeled the scattering potential of the arsenic clusters as a simple Schottky barrier potential for \( r_0 \leq r \) and as a constant potential of \( V(r) = \phi_b \) for \( 0 \leq r \leq r_0 \) as given in equation 19. Using this potential it was possible to calculate a relaxation time for arsenic cluster scattering using equation 20, and subsequently, mobility versus channel carrier concentration curves could be calculated. (For simplicity, the potential described by equation 19 will be referred to as the Schottky potential and the potential used to arrive at equation 18 will be referred to as the spherical potential for the remainder of this discussion.)
A comparison of the mobility limited by arsenic cluster scattering versus channel carrier concentration for the spherical and Schottky potentials is shown in figure 5.8. Both of the curves in figure 5.8 were calculated assuming cluster densities $N_{cl} = 10^{16}/\text{cm}^3$, a cluster radius $r_0 = 25\text{Å}$, and a concentration of ionized impurities in the channel $N_{ii} = 10^{18}/\text{cm}^3$. From this figure it can clearly be seen that the curve for the Schottky potential exhibits a much larger dependence upon the channel carrier density than does the curve for the spherical potential. This would seem to indicate that the Schottky potential should be a much better fit to the experimental data, due to the fact that the experimental data also exhibit a large dependence upon channel carrier density. Since the extent of the Schottky potential is much greater than the extent of the spherical potential, it is expected that the

![Graph showing mobility limited by arsenic cluster scattering versus channel carrier density calculated using spherical and Schottky scattering potentials.](image)

**FIGURE 5.8**
Mobility limited by arsenic cluster scattering versus channel carrier density calculated using spherical and Schottky scattering potentials.
scattering from the Schottky potential should be greater than that from the spherical potential, and thus the mobility calculated using the Schottky potential should be lower than that calculated using the spherical potential. The curves in figure 5.8 do demonstrate this effect since the mobility for the Schottky potential is much lower than the mobility for the spherical potential, even though the same simulation parameters were used.

Since it was evident from the curves in figure 5.8 that the Schottky potential model gave reasonable results, the program was run several times systematically varying the cluster radius, density of clusters and density of ionized impurities in the LT-GaAs channel region in order to find a best fit to the data in figure 5.5. The results of this calculation are shown in figure 5.9 along with the experimental data and the results obtained with the original program. The best fit for the measured data using the Schottky barrier potential was obtained for a cluster density $N_{el} = 2 \times 10^{16}/cm^3$, density of ionized impurities in the

![Graph showing mobility versus channel carrier density for spherical and Schottky potentials, with experimental data points.](image)

**FIGURE 5.9**

Mobility versus channel carrier density from calculations using a spherical potential or a Schottky potential and experimentally measured mobility data.
LT-GaAs channel region $N_{ii} = 1 \times 10^{17}/\text{cm}^3$, and an arsenic cluster radius of 30Å. All other parameters remained the same as those used in calculating the curve in figure 5.7. Although these parameters are somewhat different from those used in the calculation of Figure 5.7, they are still well within the range of observed values for this material. In Figure 5.9, it can be seen clearly that the curve calculated using the Schottky potential gives a much better fit than the curve calculated using the spherical potential. This would tend to support the theory that the arsenic clusters act like Schottky barriers within LT-GaAs layers.

The computer simulation using the Schottky potential was also run using the parameters given above and a temperature of 300K. The computer program yielded a mobility of ~1500cm$^2$/Vs at 300K compared with a measured mobility of 750cm$^2$/Vs at 300K for this sample. The fact that the program yields a 300K mobility which is too large indicates that the scattering at 300K is underestimated. This can most likely be attributed to the invalidity of the relaxation time approximation for polar optic phonon scattering at a temperature of 300K and to the fact that in-scattering for polar optical phonons was not included in this program (Negligible errors are introduced by neglecting in-scattering at 77K, but at 300K these errors are no longer insignificant.). Although the agreement of the Schottky barrier simulation results with the data is quite good, it should be possible to further refine the model in order to yield better results either by using a more descriptive scattering potential for the arsenic clusters or by using a more rigorous numerical approach.
5.8 Modulation Doped LT-GaAs Photodetector.

The large light sensitivity of the LT-GaAs MODFET structure makes it a good candidate for photodetector applications. In order to investigate the usefulness of the light sensitivity of this material, several metal-semiconductor-metal (MSM) type of photodetectors were fabricated on the LT-MODFET material. The LT-MODFET

![Diagrams of photodetector structures](image)

**FIGURE 5.10**
MSM photodetector structure for a) Ni/AuGe/Au ohmic contact on modulation doped LT-GaAs material, b) Ti/Au Schottky contact on bulk LT-GaAs material.
material was fabricated into photodetectors by photolithographically producing an
interdigitated pattern consisting of 20 fingers (5\(\mu\)m width, 5\(\mu\)m spacing, and 200\(\mu\)m
length) of Au-Ge-Ni alloyed ohmic contacts to form the source and drain contacts. These
devices, henceforth referred to as modulation doped photodetectors or MODPDs, were
then characterized to determine their spectral responsivity and current voltage
characteristics. For comparison, similar interdigital structures were fabricated with the
same mask set using a Ti-Au Schottky metalization on a 2.0\(\mu\)m thick layer of LT-GaAs
grown at 300°C and annealed in-situ in the MBE system. These detectors are shown
schematically in figure 5.10.

The operation of the MODPD is essentially the same as the operation of the LT-
MODFET discussed earlier, but a brief summary is presented again for clarity. Carriers
are transferred from the wide bandgap AlGaAs doping layer into the LT-GaAs channel
region by the normal modulation doping effect. Due to the large number of traps present
in the LT-GaAs layer, these transferred carriers are trapped, establishing a negative space
charge region in the LT-GaAs channel, rather than the usual 2-DEG formed in a normal
MODFET structure. The space charge in the LT-GaAs channel in conjunction with the
charge due to ionized impurities in the AlGaAs layer lead to pronounced band bending and
a band structure similar to a normal MODFET, with a built in field perpendicular to the
heterojunction interface. In the dark, the LT-MODFET material is extremely resistive, but
in the presence of light, the resistivity drops dramatically. It is speculated that electrons
photogenerated in the LT-GaAs layer are forced to drift to the heterojunction interface by
the built in field present in this material, where they form a conducting channel (see figure
Photogenerated holes are either trapped in the LT-GaAs material or swept away from the heterojunction interface.

This charge separation by the built in field gives rise to two mechanisms for gain in the device. The electrons which drift to the heterojunction interface and collect in the channel have a relatively long recombination lifetime ($\tau_i$) with the holes trapped in the LT-GaAs due to the spatial separation and energy barrier involved. The source to drain

\[
\begin{align*}
\text{hv} & \\
\text{DRAIN} & \\
\text{N-\text{L GaAs: Si}} & \\
\text{AuGe Ohmic Contact} & \\
\text{N+ AlGaAs: Si} & \\
\text{Contact} & \\
\text{A I GaAs q3acer - Undoped} & \\
\text{2-DEG} & \\
\text{Low Temperature GaAs} & \\
\text{GaAs Buffer Laver - Undoped} & \\
\text{Sr GaAs Substrate} & \\
\end{align*}
\]

**FIGURE 5.11**

Band structure and schematic cross-section of a MODPD.
transit time ($\tau_r$) of these electrons is thus much shorter than their recombination lifetime with the holes, giving rise to the usual photoconductive gain ($\tau_i/\tau_r$). As will be discussed shortly, these detectors also exhibit a strong light sensitivity to sub-bandgap illumination. This sensitivity to sub-bandgap illumination is believed to be due to internal photoemission from the arsenic clusters present in the LT-GaAs layer. The carriers photogenerated by sub-bandgap illumination have a long lifetime before they are re-trapped by the defects, and this again gives rise to a similar photoconductive gain ($\tau_i/\tau_r$).

The second mechanism for gain in these devices is related to the open circuit photovoltage that may be developed by the accumulation of free holes away from the heterojunction interface. The accumulation of holes will act as a positive bias applied to backgate of the device and thus will yield a drain current. This is similar to the mechanism proposed to describe the gain in MESFET photodetectors arising from the photovoltage developed at the front Schottky gate [69]. In order to establish the relative importance of each of these mechanisms, temporal/frequency measurements need to be performed.

The I-V characteristics of a typical MODPD with a LT-GaAs layer grown at 300°C is shown in figure 5.12 on the following page. The different curves in this figure are for different power levels of illumination by a white light source (a tungsten microscope illuminator was used for the light source). This figure clearly illustrates the large light sensitivity of this device. The striking similarity between these device curves and the device curves of a normal electrically gated transistor is clearly evident. These device curves exhibit a relatively linear dependence upon bias voltage when the bias is less than about 1.5 volts. For biases greater than 1.5 volts, the characteristics begin to
saturation, and at a bias of approximately 2.5 volts exhibit strong saturation. The curves show little increase in current with applied bias for voltages greater than 2.5 volts and remain relatively flat over the range from 2.5 to 20 volts.

The I-V characteristics of an MSM photodetector fabricated on a bulk layer of LT-GaAs are shown in figure 5.13. Although this device also exhibits reasonable sensitivity to light, the sensitivity of this device is clearly much smaller than that of the MODPD. Since both these devices were fabricated using the same mask set, and therefore have the same device area, the data in figures 5.12 and 5.13 can readily be compared. From figures 5.12 and 5.13 it can be seen that given similar levels of illumination, the current through the
MODPD is almost three orders of magnitude larger than the current through the MSM detector fabricated on bulk LT-GaAs. The shape of the curves in figure 5.13 are also quite different than those in figure 5.12. The characteristics of the MSM detector on bulk LT-GaAs exhibit no saturation effect with increasing bias level, even for voltages as large as 20 volts, unlike the MODPD characteristics which strongly saturate at a voltage of about 2 volts.

The spectral responsivity curves for a MODPD and an MSM device in the wavelength range from 0.7 μm to 1.4 μm are shown in Figure 5.14. Both the MODPD and MSM detectors show a sharp drop in responsivity for wavelengths greater than 0.87 μm, which corresponds to the bandedge of GaAs. The peak responsivity of the MSM photodetector on bulk LT-GaAs, which occurs at ~ 0.87 μm, is only 0.2 A/W for a 10 V

![Graph](image_url)

**FIGURE 5.13**
I-V characteristics for an MSM photodetector on bulk LT-GaAs.
bias. The peak responsivity of the MODPD, on the other hand, is an impressive 65 A/W at a bias of 1 V. The MODPD device also exhibits a large sub-bandgap responsivity of 6 A/W at a wavelength of 1.0 μm. The sub-bandgap responsivity of the MSM detector; however, is only 0.01 A/W at a wavelength of 1.0 μm, which is significantly less than that of the MODPD. The large sub-bandgap responsivity of the MODPD is also greater than the reported responsivity of 1.3 μm p-i-n photodetectors using GaAs [52], and is among the largest ever reported for a GaAs based device.

Although the MODPD has an extremely large responsivity to both bandgap and sub-bandgap light, it is also important to assess the speed at which the device can operate. In order to investigate the frequency response of the MODPD, preliminary measurements

![Graph showing spectral responsivity of MODPD and MSM photodetector.](image)

**FIGURE 5.14**
Spectral responsivity of a MODPD and an MSM photodetector.
were made using a 680 nm laser diode operated in a pulsed mode. The laser diode was
driven with a variable frequency square wave generator. The overall gain of the MODPD
was calculated by normalizing the MODPD response to the response of a germanium p-i-n
photodetector. These measurements showed that the responsivity of the MODPD
dropped off sharply at a few kHz and had lost a large portion of its gain at a frequency of
10kHz. This rapid drop in responsivity as a function of frequency is somewhat
unexpected, since p-i-n photodetectors using LT-GaAs in their active layers are among the
fastest detectors reported. The exact origin of this rapid decrease in responsivity as
frequency increases is not known at this time, but it is speculated that it may be due to the
large recombination lifetime of the photogenerated electrons in the channel and the holes
trapped in the LT-GaAs layer. Further measurements are needed to ascertain the origin of
this rapid decrease in responsivity with increasing frequency, so that the MODPD can be
optimized to overcome this serious response limitation. The frequency dependence of the
MODPD to sub-bandgap light has not yet been characterized, but similar measurements
using a 1.3 μm laser diode will be performed in the future.
5.9 Photoluminescence Measurement Results.

Photoluminescence (PL) measurements were performed using a Jarrel-Ash 0.5m monochromator system. The excitation source was the 488 nm line of an Ar$^+$ laser at a typical power density of $\sim$1W/cm$^2$. The PL signal from the sample was detected by a liquid nitrogen cooled photomultiplier tube with Si cathode and a lock-in amplifier. The reference signal for the lock-in amplifier was provided by the output of the 670 Hz beam chopper used to chop the incident laser beam.

The excess carrier recombination lifetime in LT-GaAs is extremely short (~1ps), [13,14] and the recombination process in LT-GaAs is found to be predominantly nonradiative, since no photoluminescence was observed in initial studies of the material.

![Figure 5.15](image)

**FIGURE 5.15**
Photoluminescence from a typical LT-MODFET structure.
However, more recent studies have reported weak PL lines arising from hot carriers injected by picosecond excitation, and a large number of sharp lines arising from arsenic interstitial (Asₐ) related defects and their phonon replicas.

Although only weak photoluminescence has been observed previously in bulk layers of LT-GaAs, the results of PL measurements performed at 25K on this novel LT-GaAs MODFET structure show a new PL line at 1.65eV. This feature can clearly be seen in the typical photoluminescence spectra of a LT-MODFET structure shown in figure 5.15. The smaller peak observed in this figure at ~1.8eV is due to the bandgap transition in the AlGaAs barrier layers of this device. Therefore, the position of the new PL feature is clearly at an energy which is significantly larger than the bandgap of GaAs and significantly lower than the bandgap of the AlGaAs barrier layers used in this structure. It is thus proposed that this PL line can be attributed to a spatially indirect transition from a

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**FIGURE 5.16**

Band structure and schematic diagram showing the origin of the photoluminescence peak observed in the LT-MODFET structure.
two-dimensional electron gas in the LT-GaAs at the heterojunction interface to the holes generated in the AlGaAs barrier layers

It is speculated that carriers photogenerated within the LT-GaAs channel region of this device drift to the heterointerface where they form a 2-DEG. Therefore, under constant illumination, there will be a steady state population of electrons confined at the heterojunction of the LT-MODFET device. Due to the fact that the quantum confining potential barrier at this interface is not infinite, the wavefunction of the 2-DEG will have some finite penetration into the AlGaAs layers, as is shown schematically in figure 5.16. Therefore, the carriers confined in the region of the wavefunction which penetrates into the AlGaAs layers can recombine with the holes generated in the AlGaAs layers leading to a weak photoluminescence feature. The relative energy separation of the new photoluminescence peak from the band edge peaks of AlGaAs and GaAs is in good agreement with the energy of such a transition. With the exception of a small correction due to the electron confinement energy in the well and possibly a correction for the binding energy of holes to the shallow acceptors in AlGaAs, the energy of such a transition can be given by \( E_{PL} = E_g(AlGaAs) - \Delta E_c \), where \( E_g(AlGaAs) \) is the band gap of AlGaAs and \( \Delta E_c \) is the conduction band discontinuity between AlGaAs and LT-GaAs. Assuming \( \Delta E_c = 0.6 \Delta E_g \) as is currently accepted for the AlGaAs/GaAs system [70], and assuming that the bandgap of LT-GaAs is the same as that of normal GaAs, this equation gives a value of 1.63eV for \( E_{PL} \). This value matches very well with the experimental value of 1.65 eV within the error limits previously mentioned.
It is also observed that the 1.65 eV PL line is not seen in the LT-GaAs MODFET structures after hydrogenation at 250°C for one hour. This supports the proposed model for the origin of this PL line. Hydrogen passivation of donors in different materials is well documented.[71] In the LT-GaAs MODFET structure, the neutralization of donors in the AlGaAs would lead to the removal of the space charge region in the LT-GaAs and the associated built in field and hence there would be no formation of a 2-DEG at the heterointerface under photo-excitation. This is consistent with our belief that the photogenerated 2-DEG present at the heterointerface plays a strong role in the origin of the new 1.65 eV PL line in these structures.

Recent experiments by Subramanian, Sinha and Arora at Tata Institute of Fundamental Research in Bombay India have shown Franz Keldish Oscillations (FKO) in the photoreflectance spectra obtained from these samples. The FKO in the photoreflectance spectra indicate that there is a large field present at the heterointerface in these structures, and that the magnitude of the experimentally measured field is consistent with the magnitude of the fields obtained from these structures by self-consistent calculations. This data also supports our model of the formation of a 2-DEG at the heterointerface under photo-excitation. Further support for this explanation is expected to come from future experiments to determine the effect of the mole fraction of AlGaAs in the barrier layers on the energy of the new PL feature, and Schubnikov-de-Haas oscillation measurements.
5.10 Summary of Results.

This section of this work has presented the first study of the Hall mobility of a two-dimensional electron gas (2-DEG) in MBE-grown LT GaAs using a novel MODFET device structure in which the channel region is made of LT-GaAs and all other layers are grown at normal temperatures. In the dark, the resistivity of this material was found to be extremely large, just as in bulk layers of LT-GaAs. However, when this new structure was illuminated, its resistivity became significantly lower than that of single layers of LT-GaAs, allowing reliable Hall measurements to be performed even at temperatures as low as 77K. To understand the significance of the Hall measurements more fully, theoretical values of the low field mobility of a 2-DEG in LT-GaAs were calculated from the solution of the Boltzmann equation under a relaxation time approximation by taking into account the relevant scattering mechanisms. A first order approximation for the scattering due to the presence of arsenic clusters in the LT-GaAs was implemented for the first time in this calculation. The results of this calculation, which were discussed in section 5.5, were found to be in good agreement with experimental results.

Although only weak photoluminescence had been observed previously in bulk layers of LT-GaAs, the results of PL measurements performed at 25K on this novel LT-GaAs MODFET structure showed the presence of a new PL line at 1.65eV. The position of this new PL feature was found to be at an energy which is significantly larger than the bandgap of GaAs and significantly lower than the bandgap of the AlGaAs barrier layers used in this structure. We have proposed that this new PL line can be attributed to a spatially indirect transition from the two-dimensional electron gas present in the LT-GaAs
at the heterojunction interface to the photogenerated holes present in the valence band of the AlGaAs barrier layers.

Due to the extremely large light sensitivity which was exhibited by the LT-GaAs MODFET structure, the possibility of using this material for photodetector applications was investigated by fabricating interdigitated metal-semiconductor-metal (MSM) photodetectors on the LT-GaAs MODFET structure. MSM detectors fabricated using a Ni/AuGe/Au ohmic contact metalization exhibited an excellent responsivity of 65A/W at ~0.87µm and 6.5A/W at ~1.0µm. These values of responsivity are among the highest reported for a GaAs based photodetector at this time and indicate that this device may be promising for applications requiring high sensitivity, especially in the 1.3 µm range. Present results have indicated that the speed of these devices is much lower than that of LT-GaAs P-i-N photodetectors and Schottky barrier MSM photodetectors fabricated on bulk LT-GaAs. Further work is ongoing to study the speed response of these devices more fully in order to better understand this new structure.

In the three sections of this work, results were presented to improve the fundamental understanding of the growth and material properties of several important materials used in MODFET and opto-electronic devices. The first section addressed the use of carbon as a p-type dopant in III-V semiconductors. The second section addressed the effects of substrate temperature on the growth and properties of InGaAs and the third section addressed the use of a novel MODFET structure to study the properties of GaAs grown at low temperatures. Each of these sections provided several important results which are summarized below.

The first section studied the effect of substrate orientation upon the material properties of MBE grown carbon doped GaAs. Samples were grown on (100), (111A), and (111B) orientated substrates with doping levels varying from approximately $10^{17} \text{/cm}^3$ to $10^{20} \text{/cm}^3$. Van der Pauw Hall measurements showed all samples were p-type regardless of substrate orientation, and the mobility measured in the carbon samples was found to be comparable to similar beryllium doped samples. In contrast to silicon which exhibits strong amphoteric behavior and can produce either n or p-type doping depending upon substrate orientation and growth conditions, we have found no similar substrate dependence or strong amphoteric behavior for carbon doping in GaAs. At high carbon doping levels ($p>5 \times 10^{19}/\text{cm}^3$) the PL spectrum from carbon doped samples showed an additional peak which is believed to be associated with a transition from the conduction band to light hole valence band.
In the second section the effects of substrate temperature upon the growth and material properties of InGaAs were studied. In this work, we have found that bulk inter-diffusion processes play an important factor in the formation of the InGaAs/GaAs interface and even more so in the formation of the InGaAs/AlGaAs interface. An increased indium reevaporation at about 565°C was found to coincide with the phase transition of the surface reconstruction from As stabilized to metal stabilized and is caused by arsenic limited incorporation of indium. It was also demonstrated in this section that the quality of InGaAs/AlGaAs materials could be greatly improved by growing the layers at relatively high substrate temperature (~570°C) and inserting a GaAs spacer between the two layers.

The final result of this section posed several interesting questions which still have not been totally resolved. In several samples Auger analysis determined that a small amount of indium was present on the surface of samples even though a 1000Å overlayer of GaAs or AlGaAs was grown over the InGaAs quantum well. This result may indicate that either bulk outdiffusion from the InGaAs quantum well or segregation of a small surface layer of indium occurs during overlayer growth. In order to assess which of these theories is correct, depth profiles of the samples should be done using either Auger or SIMS to determine if the indium is only present on the surface (indicating that a thin layer of indium segregates on the sample surface during growth but does not incorporate into the bulk of the overlayer) or whether there is indium present throughout the 1000Å overlayer (indicating that indium must be diffusing from the bulk of the well during the growth of the overlayer). Unfortunately at the time of this work, these experiments could
not to be performed, but these experiments would be a good addition to the results provided in this section and a valuable use of time for someone wanting to explore this work further.

The third section of this work described the growth, fabrication and measurement of a novel MODFET structure in which the channel region was made of GaAs grown at low substrate temperatures and all other layers were grown at normal temperatures. This novel MODFET structure provided us with the ability to perform the first study of the Hall mobility of a two-dimensional electron gas (2-DEG) in MBE-grown LT GaAs. In the dark, the resistivity of this material was found to be extremely large, just as in bulk layers of LT-GaAs. However, when this new structure was illuminated, its resistivity became significantly lower than that of single layers of LT-GaAs, allowing reliable Hall measurements to be performed even at temperatures as low as 77K.

To understand the significance of the Hall measurement results obtained from the LT-GaAs MODFET structure more fully, theoretical values of the low field mobility of a 2-DEG in LT-GaAs were calculated from the solution of the Boltzmann equation under a relaxation time approximation by taking into account the relevant scattering mechanisms. A first order approximation for the scattering due to the presence of arsenic clusters in the LT-GaAs was implemented for the first time in this calculation. The results of this calculation, which were discussed in section 5.6, were found to be in good agreement with experimental results.

Although only weak photoluminescence had been observed previously in bulk layers of LT-GaAs, the results of PL measurements performed at 25K on this novel LT-
GaAs MODFET structure showed the presence of a new PL line at 1.65eV. The position of this new PL feature was found to be at an energy which is significantly larger than the bandgap of GaAs and significantly lower than the bandgap of the AlGaAs barrier layers used in this structure. We have proposed that this new PL line can be attributed to a spatially indirect transition from the two-dimensional electron gas present in the LT-GaAs at the heterojunction interface to the photogenerated holes present in the valence band of the AlGaAs barrier layers. In order to confirm or deny this hypothesis, many more experiments still need to be done, and would provide a good starting point for anyone wanting to follow this work.

Since the LT-GaAs MODFET structure exhibited an extremely large light sensitivity, the possibility of using this material for photodetector applications was investigated by fabricating interdigitated metal-semiconductor-metal (MSM) photodetectors on the LT-GaAs MODFET structure. MSM detectors fabricated using a Ni/AuGe/Au ohmic contact metalization exhibited an excellent responsivity of 65A/W at ~0.87μm and 6.5A/W at ~1.0μm. These values of responsivity are among the highest reported for a GaAs based photodetector at this time and indicate that this device may be promising for applications requiring high sensitivity, especially in the 1.3 μm range. Present results have indicated that the speed of these devices is much lower than that of LT-GaAs P-i-N photodetectors and Schottky barrier MSM photodetectors fabricated on bulk LT-GaAs. Further work is ongoing to study the response speed of these devices more fully in order to better understand this new structure.
References


