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**Effects of external perturbations on the optical properties of
semiconductor microstructures**

Qiang, Hao, Ph.D.

City University of New York, 1993

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**EFFECTS OF EXTERNAL PERTURBATIONS ON
THE OPTICAL PROPERTIES OF SEMICONDUCTOR MICROSTRUCTURES**

by

HAO QIANG

A dissertation submitted to the Graduate Faculty in
Physics in partial fulfillment of the requirement for the
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1993

This manuscript has been read and accepted for the Graduate Faculty in Physics in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy.

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Abstract**EFFECTS OF EXTERNAL PERTURBATIONS ON
THE OPTICAL PROPERTIES OF SEMICONDUCTOR MICROSTRUCTURES**

by

Hao Qiang

Advisor: Distinguished Professor Fred H. Pollak

Semiconductor microstructures have become more and more important because they have generated many types of novel devices. Optical spectroscopy is one of the most powerful tools in studying semiconductor microstructures. In this thesis, modulation spectroscopy (MS) and time resolved photoluminescence (PL) spectroscopy have been used to study the effects of external perturbations, such as temperature, electric field and uniaxial stress, on the optical properties of semiconductor microstructures.

Temperature dependence of the MS line shape, exciton transition energy and linewidth of quantum well (QW) structures have been studied. We report the experimental evidence of the reduced exciton-phonon interaction in reduced dimensional systems.

Electric field effects in semiconductor microstructures are quite different from the bulk semiconductor materials. Effects of homogeneous electric field controlled by external bias have been studied in QW and coupled double QW (CDQW) structures.

Pseudomorphic InGaAs high electron mobility transistors (HEMT) with huge built-in inhomogeneous electric field have also been studied.

Uniaxial stress is a very powerful tool for tuning the electronic band structures. Deformation potentials of AlGaAs ternary alloy materials of several Al compositions have been measured. QW structures of different material systems such as unstrained GaAs/AlGaAs, biaxially compressed InGaAs/GaAs, and biaxially tensioned GaAs/Si systems have been studied under large in-plane uniaxial stress (up to 10 ~ 20 kbar). Both the energy dependence and polarization behavior are quite different for light and heavy hole features. Phenomena related to the piezoelectric field have been observed for the low symmetry [110] stress axis. Different screening to the generated electric field has been observed among different material systems such as between InGaAs/GaAs and GaAs/AlGaAs systems. Preliminary experimental results of the growth directional stress configuration were also discussed.

Uniaxial stress influence on the dynamical properties has been studied using time resolved PL spectroscopy. Relaxation processes of free holes in a bulk n^+ -GaAs sample, excitons in an intrinsic GaAs/Si QW structure and free carriers in a p^+ -GaAs/Si QW structure have been studied.

Dedication

to Jingyan Gu

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Hao Qiang

Brooklyn, New York

August 1993

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Symbols and Abbreviations

Symbols and abbreviations frequently used in this thesis:

Symbols

α, β	Varshni thermal coefficients
α_s, β_s	Seraphin coefficients
Γ_0	Linewidth (Γ) at zero temperature
Γ_{cp}	Electron (exciton) -LO phonon coupling constant
a, b, d	Deformation potential parameters (hydrostatic, shear [001], shear [111])
k_B	Boltzmann constant
$mnH(L)$	Denotes quantum transition from mth conduction band to nth HH(LH) valence band. The HH or LH mass convention throughout this thesis is determined along the (001) growth direction.
E_{LO}	Zone center LO phonon energy
E_0	Fundamental direct band gap
F	Electric field
L_z	Well width of quantum well structure
S	Uniaxial stress
T	Temperature

abbreviations

2DEG	Two Dimensional Electron Gas
CDQW	Coupled Double Quantum Well
EBER	Electron Beam Electorelectance
EER	Electrolyte Electorelectance
EM	Electromodulation
ER	Electorelectance
FDGL	First Derivative Gaussian Lineshape
FDLL	First Derivative Lorentzian Lineshape
FKO	Franz-Keldysh Oscillation
HEMT	High Electron Mobility Transistor
HH	Heavy Hole
LH	Light Hole
LO	Longitudinal Optical (phonon)
LPE	Liquid Phase Epitaxy
MBE	Molecular Beam Epitaxy

MDQW	Modulation Doped Quantum Well
ML	Monolayer
MOCVD	Metallo-Organic Chemical Vapour-phase Deposition
MS	Modulation Spectroscopy
MQW	Multiple Quantum Well
NID	Non-Intentional Doping
PL	Photoluminescence
PLE	Photoluminescence Excitation
PR	Photoreflectance
PzR	Piezoreflectance
SL	Superlattice
SQW	Single Quantum Well
QW	Quantum Well

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EFFECTS OF EXTERNAL PERTURBATIONS ON THE OPTICAL PROPERTIES OF SEMICONDUCTOR MICROSTRUCTURES

Chapter 1. Introduction

This work involves both experimental and theoretical research on optical properties of semiconductor microstructures. The organization of this thesis is as following:

In Chapter 2, some general background knowledge will be discussed. Three key elements of this thesis as depicted in Fig. 1, namely semiconductor microstructures(SM), modulation spectroscopy(MS), and external perturbations(EP), will be discussed in three separate subsections. Chapter 3 is the theoretical background concerning the modulation spectroscopy method, such as the modulation mechanism and the appropriate line shape functions.

Various theoretical calculation methods of treating external/internal perturbations used in this work are summarized in Chapter 4 for readers who are interested in the detailed underlying theory and calculation methods.

Chapters 5, 6, 7, and 8 are devoted to our experimental findings about temperature, electric field, and uniaxial stress effects (both static and dynamic properties), respectively. In each chapter, there will be first a brief introduction,

followed by a brief description of the experimental setup. Then, various experimental results will be presented as well as discussions where necessary. In the end, for the ease of readers, I will make a brief summary. Readers are referred to the introduction and summary parts of these sections to find out their contents.

Finally, I will make some conclusions in addition to suggestions of future works in Chapter 9. Listed in Appendix A are my publications during the course of this work. After appendix is the bibliography.

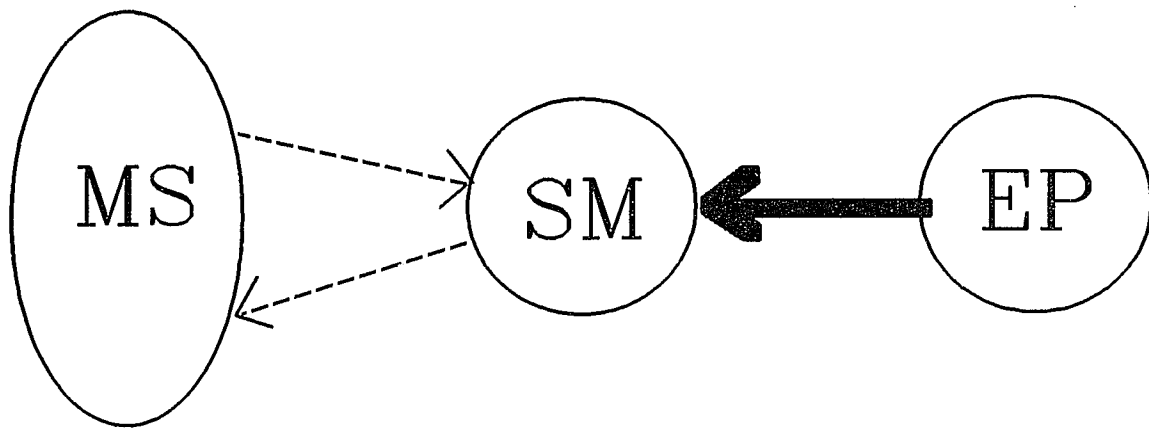


FIG. 1 Three key components of this work and their schematic relationship.

Chapter 2. Background

The object of this work is various semiconductor microstructures, the semiconductor materials with artificial structures of nanometer dimensions. We are interested in how the various properties of these semiconductor microstructures, such as the exciton transition energies and broadening parameters, change under the influence of different kinds of external perturbations. We will mainly use the high sensitive and convenient modulation spectroscopy (MS) methods. In this chapter, I will discuss briefly the background knowledge of three key components of this thesis, i.e., semiconductor microstructures, optical spectroscopy, and external perturbation as depicted in Fig. 1. In the end of this chapter, I will describe several sample preparation procedures used during this work.

2.1 Semiconductor Microstructures

We know that various properties in solid state physics originate from the distinctive long range order (symmetry property). The different periodicity together with different kinds of symmetry properties of different natural crystal materials (including semiconductor materials) produce rich variety of material properties. The *endless* search of new materials relies in large extent on the ordering (symmetry) property. After we cataloged all thirty-two symmetry groups, our knowledge was greatly improved but in the mean time we saw the *end* since our world seemed to be restricted within these finite boundaries. The classical question of why there are only thirty-two choices is now the

textbook problem for those college students in the solid state physics course. However, the search of new natural symmetry group beyond has never stopped in spite of this verdict. Recently, the five fold symmetry axis was found, and the symmetry of C_{60} was also a truly exciting event. But the most influential approach was the one suggested by Esaki and Tsu in 1969, where human factor involves more than nature. The original proposal was a *superlattice*, a novel idea of artificial structure, in which a one dimensional potential is engineered with epitaxy of alternating ultrathin layers of different properties. The new low dimensional periodicity, and its rich controllable parameters can bring us materials with properties not found in nature and controlled according to our will. With the advancement of modern material growth techniques such as molecular beam epitaxy (MBE) and metallo-organic chemical vapor-phase deposition (MOCVD), this field of research is very active and fruitful after 80s. This revolutionary idea has and will make many physicists as well as device people busy for a while.

Various low dimensional structures have been studied by different methods. For instance, single quantum well (SQW), multiple quantum well (MQW), coupled double quantum well (CDQW), superlattice (SL), high electron mobility transistor (HEMT), and recently 1D quantum wires, 0D quantum dots, etc. Beginning in the 80s, there has been considerable effort in using photoreflectance (PR) and other modulation techniques in the study of these microstructures (F. H. Pollak, 1991; Glembocki and Shanabrook, 1992). The rich modulated spectra from microstructures could be used to probe the *band structure* of reduced dimensional systems just as this optical method was employed in

bulk materials. Besides its well-known sharp derivative-like spectra yielding high resolution of and sensitivity to transition energies, other valuable information from the system can be obtained through more detailed study such as line shape analysis. Among different spectroscopy methods, modulation spectroscopy is becoming increasingly more important for studying and characterizing the microstructure properties because of the advantages which we will discuss in the following section together with its relative simplicity and ease of operation of the instrumentation.

In this work we will use QW structure in most cases since this is the simplest yet essential building block of most microstructures. We will use the notation $mnH(L)$ to denote the optical transitions from m th conduction subband to n th HH(LH) valence subband.

2.2 Optical Spectroscopy

2.2.1 A Powerful Probe

There are many ways to probe semiconductor microstructures. Optical spectroscopy is among the most valuable tools we possess today. It is an appropriate tool on probing the electronic band structures because inter/intra-subband transition energies of these semiconductor materials match the optical frequency range. Optical spectroscopy offers tools which cover almost all the interesting research areas of the semiconductor microstructures. Let's examine the Hamiltonian of these systems. In condensed matter

physics, the Hamiltonian can be in principle broken down into three parts:

$$H=H_e+H_{ph}+H_{ep} \quad (2.1)$$

where H_e , H_{ph} , and H_{ep} describe the electron system, phonon system, and interactions between them, respectively.

The first term H_e can be well described by the electronic band structures. It has been extensively studied by various theoretical approaches and experimental work. Optical spectroscopy can probe the critical point transitions directly. Examples are MS, photoluminescence (PL) spectroscopy, photoluminescence excitation (PLE) spectroscopy, ellipsometry, absorption spectroscopy, and reflectance spectroscopy, etc.

The second term H_{ph} describes lattice vibrations. The normal mode excitations are usually referred as phonons. Optical spectroscopy such as the Brillouin and Raman scattering can probe them indirectly through second order process, while the infrared reflectivity offers a direct optical probe.

The last term H_{ep} describes the interaction between the former two systems. There is relatively little work done in this area in the reduced dimensional system by optical spectroscopy method. Changes are expected to happen in going from 3D bulk materials to reduced dimensional systems such as 2D QWs due to the confinement of both electrons (excitons) and phonons. The coupling between these two systems can be probed by perturbing the electron system while monitoring the changes on the phonon

system, or vice versa. For example, the dependence of the optical transition linewidth on the phonon populations reflects directly the strength of this coupling. One convenient yet accurate way of tuning the phonon populations is by changing the lattice temperature as we will pursue in Chapter 5. Thus optical spectroscopy can also contribute to the understanding of this field.

We see, basically almost all the properties of semiconductor microstructures can be studied by optical probes. The optical spectroscopy methods, which have been used in this work, are various forms of MS, PL, PLE, and time-resolved PL. All the MS experiments were performed in Brooklyn College while the rest were through various collaborators. Therefore, I will discuss here in more detail about the MS method.

2.2.2 Modulation Spectroscopy

MS is a powerful experimental technique to study the optical properties and band structures of semiconductors and semiconductor microstructures. It produces sharp derivative like spectral features by measuring the change in optical response with respect to certain parameter of the sample or measuring system instead of the absolute response. The sensitivity of such measurements can be greatly enhanced by making full use of the advantages of phase sensitive detection with the external perturbation in a periodic fashion. The observed normalized changes are usually small so that the difference signals are closely related to a derivative of the absolute spectrum with respect to the modifying parameter. The derivative nature of MS emphasizes critical point transitions

and suppresses uninteresting background. There are various kinds of perturbations applicable to obtain MS. The conventional techniques include most popular electromodulation (EM) [*e.g.*, electroreflectance (ER), photorefectance (PR), electrolyte electroreflectance(EER), electron beam electroreflectance (EBER), etc.], piezoreflectance (PzR), temperature modulation, and wavelength modulation, etc.

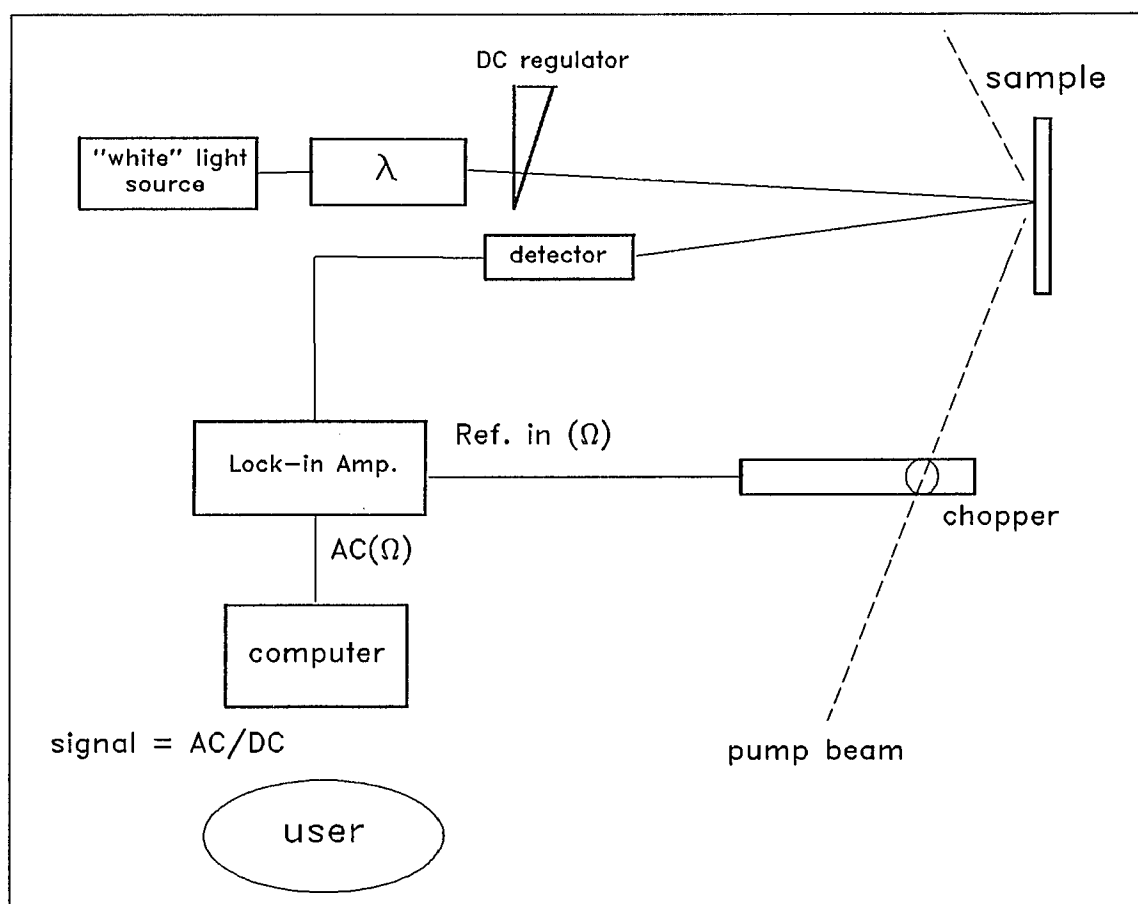


FIG. 2 Schematic diagram of a typical PR setup.

In Fig. 2, we show the schematic diagram of a typical photorefectance setup. A *white* (broad band) light source is dispersed by a monochromator. The output

monochromatic light is focused onto the investigating sample. The reflected light is collected by an appropriate optical detector, e.g. a high sensitive, low noise Si-diode detector. The lenses, mirrors and optical filters are omitted for simplicity. The photonic signal is thus transformed into an electronic signal. This optical path forms a typical reflectance spectroscopy setup. By varying the monochromatic wavelength, one will obtain an absolute reflectance spectrum R . The idea of modulation spectroscopy is trying to measure the difference ΔR instead of the absolute R in order to achieve higher signal to noise ratio as well as getting rid of the huge uninteresting background which is present in the absolute reflectance measurement. There are many ways to achieve the modulation. The modulation of PR in Fig. 2, for example, is obtained by illuminating the probing sample spot with a secondary light beam, which is typically a compact He-Ne laser. This modulating pump beam is turned on and off by a chopper system (e.g., mechanical or acoustic-optical modulator) in a periodic fashion. When the light is off, we have the normal signal R from the detector. When it is on, the signal becomes $R + \Delta R$, where ΔR is due to the pump beam perturbation. Since the pump beam is on and off with a regular frequency Ω , the ΔR will also be fluctuating between ΔR and 0 with the very same frequency. By using a phase sensitive lock-in amplifier tuned at the chopping frequency Ω , ΔR can be detected very accurately yielding high noise rejection ratio. The modulation signal is obtained through a division operation $\Delta R/R$, which can be achieved through computer digital manipulation or electrical servo system. An optical servo system was later developed to regulate the monochromator output light intensity, which was known to cause problems in the final spectrum especially when sharp spectral

lines were present in probing light sources such as an intense Xe-arc lamp. If this optical servo system is deployed, the measured ΔR will be proportional to the actual signal $\Delta R/R$.

A reflectance spectrum of GaAs at 300K is shown in Fig. 3(a). Notice the huge background on which various interesting critical point features ride. For comparison an ER spectrum of bulk GaAs taken at 300K is shown in Fig. 3(b). Now the critical point features are much enhanced. The advantages of MS over reflectance spectroscopy are clearly demonstrated in this example.

When comparing to the other popular tools such as PL, $\Delta R/R$ of MS, as inherited from absolute reflectance spectroscopy, has the advantage of richer features, especially above the fundamental absorption edge. And the difficulties due to the presence of trapping centers and nonradiative channels will be much less in relation to PL and other methods based on it such as PLE. Because MS produces sharp localized features with respect to photon energy, line shape fit with relatively simple models can be performed to yield accurate values of energy and linewidth (Γ) of the observed transitions. The precision can be within a few meV, even at room temperature. Other parameters such as intensity, broadening and phase as well as distinctive parameters like modulation frequency, in/out phase response, etc., bring about even more useful information. All these advantages of MS make it an extremely powerful method for the study of effects of static external perturbations on semiconductor microstructures.

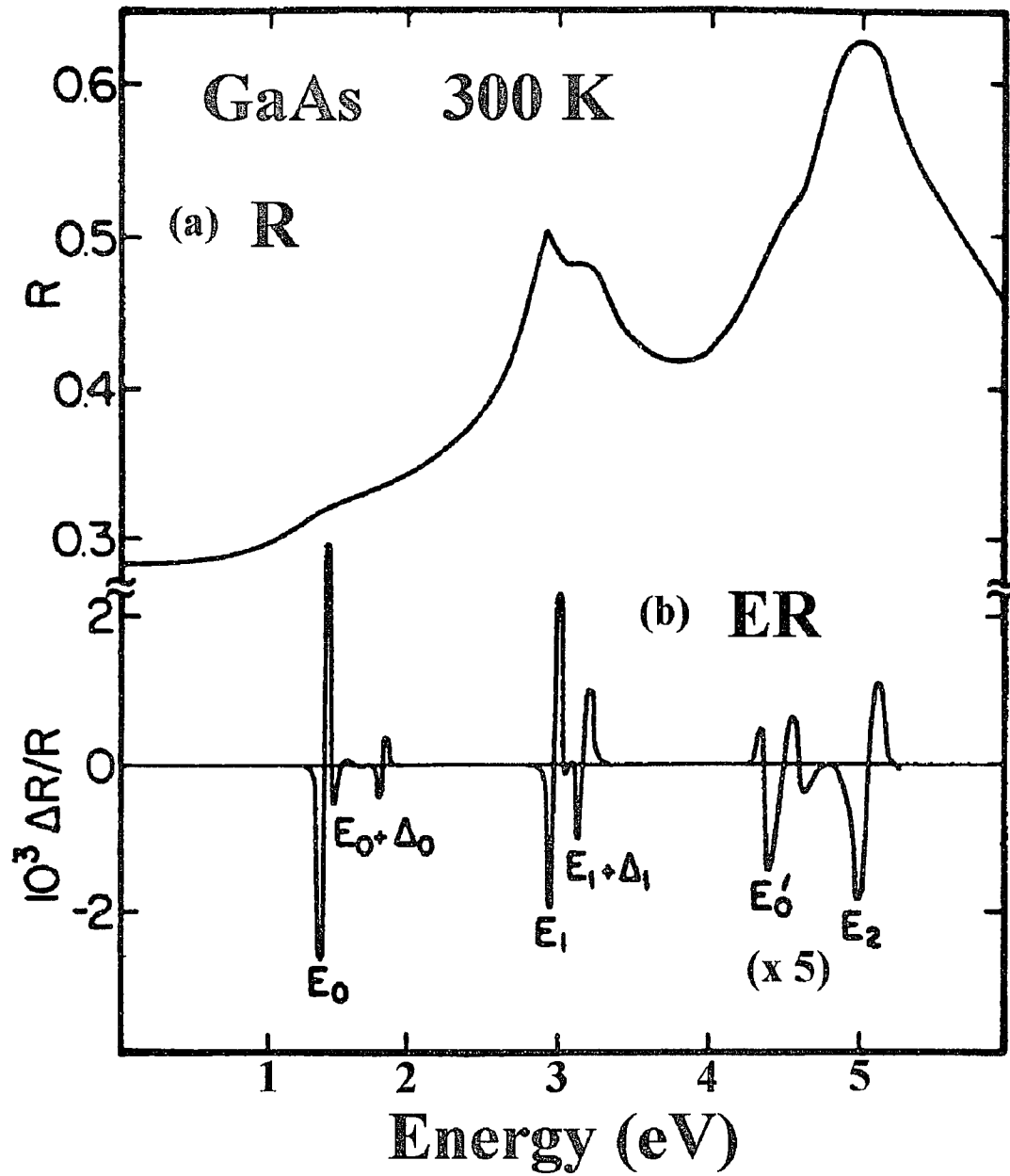


FIG. 3 (a) Absolute reflectance and (b) ER spectra of bulk GaAs at 300K.

2.3 Perturbations by External Parameters

While to characterize a unperturbed semiconductor microstructure is important, it is more important to study the quantitative dependence on various static external

perturbations of the optical and electronic properties of microstructures. All these properties themselves are interesting from the fundamental point of view. On the other hand, from the application point of view, it is based on and utilizing these knowledge that various novel devices with improved performance become reality.

The effects of static external perturbations can be conveniently studied by MS. The contactless modulation spectroscopy method of PR is particularly suitable for such study, since it has nearly no sample restrictions (see Fig. 2). Therefore, there is plenty of freedom around the sample so as to create various external environments (perturbations).

The static external perturbations that we intend to study in this work are temperature (T), electric field (F), and uniaxial stress (S). They range from scalar, vector, to tensor. We list the portrait of each of them as following:

2.3.1 Temperature (T)

It is a scalar perturbation, which preserves all the symmetry properties of the system. Its influences on electronic system are mainly changes of transition energies and level broadening. The optical transition energy shift is due to lattice expansion and electron phonon interaction. The phonon population also relies on the lattice temperature according to the Bose-Einstein distribution, and consequently the thermal broadening reveals important information about electron (exciton)-phonon interaction.

2.3.2 Electric Field (F)

It is a vector perturbation, which destroys translational symmetry along the field direction. There are many interesting effects related to the electric field, such as Stark effect, interwell coupling and decoupling between coupled wells, Wannier-Stark localization, etc. It is the most widely used control parameter in real devices.

2.3.3 Uniaxial Stress (S)

It is a second rank 3×3 tensor perturbation, usually in a reduced six-vector form for an S_4 symmetry material. It also lowers symmetry operations of a system, but unlike the electric field perturbation, the translational and inversion symmetries are always preserved. The modification to the band structures can be well described by deformation potential theory. Stress along a low symmetry axis of a polar material, e.g. GaAs, generates a piezoelectric field.

2.4 Sample Preparation

Samples used in this study are either commercial products or grown by various collaborators. They will be mentioned in their relevant usages.

Usually the surface quality of a sample is good enough as it is for our optical measurements. But there are indeed times when the surface polishing is necessary. The sample polishing is performed on a BUEHLER POLIMET polishing system. The typical treatment for a GaAs material is 30 minute 1000 grid, 1 hour $0.3\mu\text{m}$, 1 hour $0.05\mu\text{m}$,

1 hour Syton, and 1 minute 1:1 mixture of Bromine and Methanol.

In preparing the sample piece for uniaxial stress experiment, special care must be taken to avoid mechanical damages as well as to regulate sample shapes so as to achieve a high and uniform stress distribution inside a sample. The crystal orientation is determined to better than 1° by X-ray backscattering except those samples with flat edge marks available. The sample slice (typically 2mm wide and 15mm long) is cut off along the designated direction on a BUEHLER 11-1180 Low Speed Saw with the sample mounted on a rotation stage which is transferred directly from the X-ray equipment. It is then further hand ground to the desired bar shape, and polished as necessary.

Chapter 3. Modulation Spectroscopy Lineshape Consideration

As discussed in the previous chapter, modulation spectroscopy (MS) measures relative change of R with respect to certain modulating parameter instead of absolute R of a sample. This high sensitive technique produces sharp derivative like features around critical transition points where the density of states undergoes dramatic change. Besides the enhanced signal to noise ratio as well as other benefits, one direct impact on the data analysis is due to its well localized features. Even though it is very difficult to model an absolute reflectance spectrum, a localized feature in a modulation spectrum is quite simple to model accurately. This advantage makes it an accurate optical technique. In this chapter the theoretical modeling of localized MS features will be discussed and some commonly adopted ones as well as those been used in this work are discussed.

If a collimated light beam is projecting onto a flat interface between air and a homogeneous medium in a normal incidence configuration, the reflectance can be expressed as:

$$R = \left(\frac{1-n}{1+n} \right)^2 \quad (3.1)$$

where n is the complex reflectivity of the medium.

In general the reflectance R from an air-sample interface will be a more complicated function of the sample reflectivity n or equivalently the dielectric function

ϵ (or *effective* ϵ in multi-layered semiconductor microstructures).

$$R=R(\epsilon_1, \epsilon_2) \quad (3.2)$$

The normalized change of reflectivity as typically measured in a MS experiment is related to the modulated dielectric function by (D. E. Aspnes, 1980):

$$\frac{\Delta R}{R} = \alpha_s(\epsilon_1, \epsilon_2) \Delta \epsilon_1 + \beta_s(\epsilon_1, \epsilon_2) \Delta \epsilon_2 \quad (3.3)$$

where α_s and β_s are the Seraphin coefficients. The quantities $\Delta \epsilon_1$ and $\Delta \epsilon_2$ are the changes in the real and imaginary parts of the dielectric function, respectively, induced by the particular modulating parameter, e.g., electric field in ER.

3.1 Exciton Line Shape Functions

It has been show that for bound states such as excitons or the confined states of a QW, $\Delta \epsilon$ is a first-derivative spectroscopy. Thus one can write:

$$\Delta \epsilon_i = \left[\frac{\partial \epsilon_i}{\partial E_x} \frac{dE_x}{dF} + \frac{\partial \epsilon_i}{\partial \Gamma} \frac{d\Gamma}{dF} + \frac{\partial \epsilon_i}{\partial I} \frac{dI}{dF} \right] \Delta F \quad (3.4)$$

or

$$\Delta \epsilon_i = [A_x f_x^{(i)}(y) + A_\Gamma f_\Gamma^{(i)}(y) + A_I f_I^{(i)}(y)] \left(\frac{I \Delta F}{\Gamma} \right) \quad (3.5)$$

where:

$$A_x = \frac{1}{\Gamma} \frac{dE_x}{dF} \quad A_\Gamma = \frac{1}{\Gamma} \frac{d\Gamma}{dF} \quad A_I = \frac{1}{I} \frac{dI}{dF} \quad y = \frac{E - E_x}{\Gamma} \quad (3.6)$$

In the above equations, E_x is the exciton energy, Γ is the broadening parameter, I is the integrated intensity, while script i denotes the real ($i=1$) or imaginary ($i=2$) part. The quantities $f_x^{(i)}(y)$, $f_\Gamma^{(i)}(y)$, and $f_I^{(i)}(y)$ are the appropriate line shape functions corresponding to the modulation of the exciton energy, broadening, and intensity, respectively. F is the modulating parameter (e.g. electric field in ER).

Combining these equations, we have the general line shape model:

$$\begin{aligned} \frac{\Delta R}{R} &= [S] \times [L] \times [A] \\ &= (\alpha_s \quad \beta_s) \begin{bmatrix} f_x^{(1)}(y) & f_\Gamma^{(1)}(y) & f_I^{(1)}(y) \\ f_x^{(2)}(y) & f_\Gamma^{(2)}(y) & f_I^{(2)}(y) \end{bmatrix} \begin{bmatrix} A_x \\ A_\Gamma \\ A_I \end{bmatrix} \end{aligned} \quad (3.7)$$

The first matrix $[S]$ is the Seraphin coefficients, which is the "sample matrix". The third matrix $[A]$ is the modulating amplitude of E_x , Γ , and I , which can be called "modulating matrix". The second matrix $[L]$, "line shape matrix", consists of six line shape functions. The "sample matrix" and "modulating matrix" can and can only be modified by changing the sample structure and modulating method, respectively. $[S]$ can be in principle evaluated from the detailed knowledge of the sample system. $[A]$ can be significantly different between different modulation techniques, such as the PR and PzR. Because of the well localized nature of modulation spectroscopy, $[S]$ and $[A]$ are practically treated as constants for a feature. The "line shape matrix" $[L]$ is more universal. We will concentrate here on the "line shape matrix".

For excitons the dielectric function will have either a Lorentzian or Gaussian profile depending on whether the broadening is homogeneous or inhomogeneous, respectively. For the case of First Derivative Lorentzian Lineshape (FDLL) the dielectric function and the corresponding line shape functions can be expressed as:

$$\epsilon = 1 + \frac{I}{E - E_x + i\Gamma}$$

$$[L] = \begin{bmatrix} -\frac{1-y^2}{(1+y^2)^2} & -\frac{2y}{(1+y^2)^2} & \frac{y}{1+y^2} \\ -\frac{2y}{(1+y^2)^2} & \frac{1-y^2}{(1+y^2)^2} & -\frac{1}{1+y^2} \end{bmatrix} \quad (3.8)$$

For the case of First Derivative Gaussian Lineshape (FDGL), the dielectric function is:

$$\epsilon = 1 + I(L_1 + iL_2) \quad (3.9)$$

where a Gaussian profile of ϵ_2 is given by:

$$L_2 = \frac{B}{\Gamma} e^{-Cy^2} \quad (3.10)$$

here we choose $C = \ln 2 \approx 0.693$ so that the half-width at half maximum (HWHM) of ϵ_2 is Γ , and $B = -1$ so that peak value of $\epsilon_2(E = E_x) = -I/\Gamma$. This is different from the previous definition ($C = 1$), but it is more consistent with the definition of FDLL.

From the Kramers-Kronig relation, we have:

$$L_1 = 2 \sqrt{\frac{C}{\pi}} \frac{y}{\Gamma} \phi\left(1, \frac{3}{2}, -Cy^2\right) \quad (3.11)$$

where ϕ is the confluent hypergeometric function.

The appropriate line shape functions are thus obtained by taking derivatives:

$$[L] = \begin{bmatrix} -2\sqrt{\frac{C}{\pi}}\phi\left(1, \frac{1}{2}, -Cy^2\right) & -4\sqrt{\frac{C}{\pi}}y\phi\left(2, \frac{3}{2}, -Cy^2\right) & 2\sqrt{\frac{C}{\pi}}y\phi\left(1, \frac{3}{2}, -Cy^2\right) \\ -2Cye^{-Cy^2} & (1-2Cy^2)e^{-Cy^2} & -e^{-Cy^2} \end{bmatrix} \quad (3.12)$$

The line shape functions are plotted in Fig. 4 and Fig. 5 for the case of FDLL and FDGL, respectively. Generally speaking, the FDGL has pronounced "wings" for $f_x^{(i)}$ and $f_\Gamma^{(i)}$ as compared to the FDLL case.

In order to fit the experimental data with the theoretical model discussed above, we need 6 independent fitting parameters (E_x , Γ , ratio of α_s/β_s , A_x , A_Γ , and A_I) for each peak. In actual practice, we will usually neglect the intensity modulation since only E_x and Γ modulations have been shown to be important (F. H. Pollak and O. J. Glembocki, 1988) in the low field region. Thus we need four parameters, i.e., E_x , Γ , $\theta = \tan^{-1}(\beta/\alpha)$, and $\varphi = \tan^{-1}(A_\Gamma/A_x)$, in its normalized form:

$$\frac{\Delta R}{R} \propto (\cos\theta \quad \sin\theta) \begin{bmatrix} f_x^{(1)}(y) & f_\Gamma^{(1)}(y) \\ f_x^{(2)}(y) & f_\Gamma^{(2)}(y) \end{bmatrix} \begin{bmatrix} \cos\varphi \\ \sin\varphi \end{bmatrix} \quad (3.13)$$

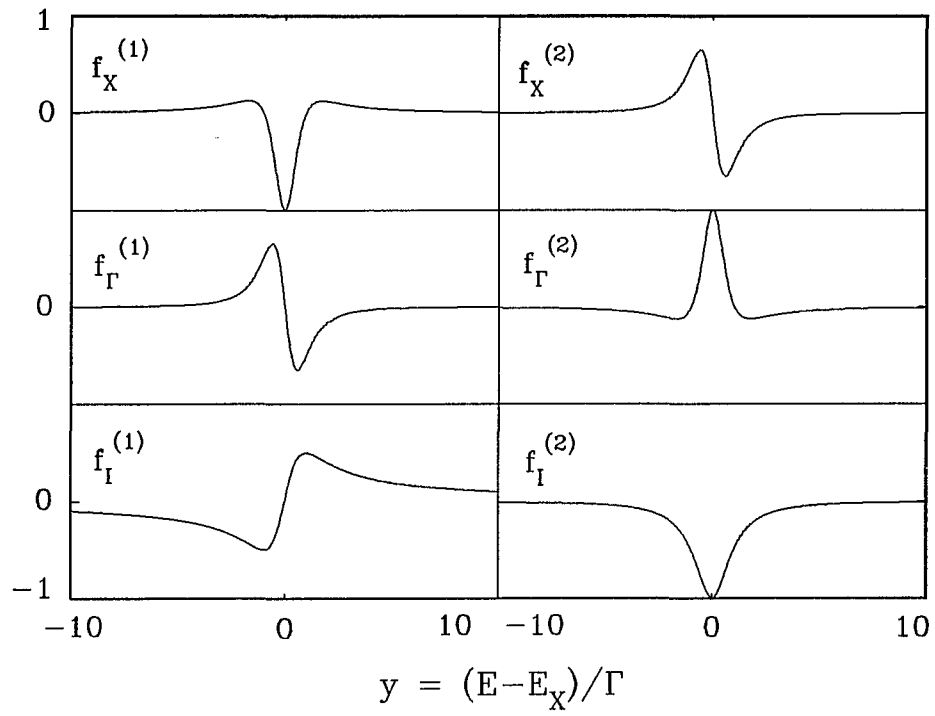


FIG. 4 Line shape functions of FDLL.

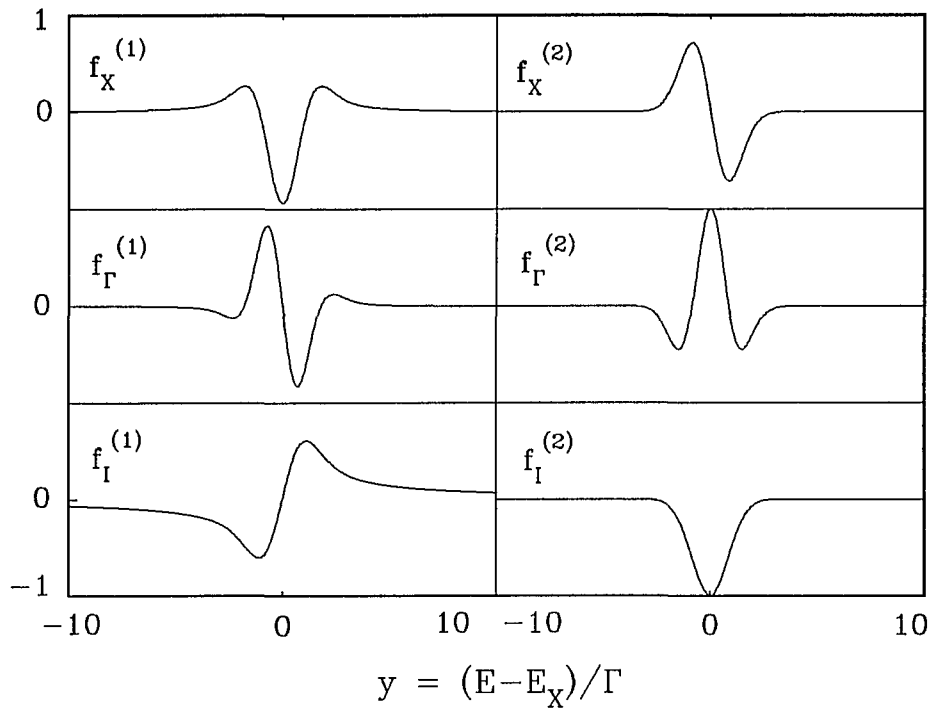


FIG. 5 Line shape functions of FDGL.

For the case of FDLL, because of its analytical properties, $f_x^{(1)} = -f_\Gamma^{(2)}$ and $f_x^{(2)} = f_\Gamma^{(1)}$, the fitting parameters can be further reduced to three as:

$$\frac{\Delta R}{R} \propto \cos \Omega f_x^{(1)}(y) + \sin \Omega f_x^{(2)}(y) \quad (3.14)$$

where $\Omega = \theta + \varphi$. Or, since $f_x^{(1)} + i f_x^{(2)} = [\Gamma / (E - E_x + i\Gamma)]^2$, this can equivalently be written as the one proposed by Aspnes (1980):

$$\frac{\Delta R}{R} \propto \text{Re}[e^{i\Omega}(E - E_x + i\Gamma)^{-n}] \quad (3.15)$$

with $n=2$ for exciton.

Some early work suggested similar reduction of parameters to FDGL so that $f_x^{(2)}$ and $f_\Gamma^{(2)}$ are approximated by $f_\Gamma^{(1)}$ and $f_x^{(1)}$, respectively. This procedure may yield correct E_x and even Γ , but the "wing" structures can not always be reproduced correctly.

3.2 Unbound Band-to-Band Critical Point Transitions

For unbound band-to-band critical point transitions, modulation spectroscopy yields either a first or a third derivative spectrum (F. H. Pollak and

Table I Values of power n in line shape function [Eq. (3.15)] for various critical points.

	First Derivative	Third Derivative
2D	1	3
3D	0.5	2.5
Exciton	2	N/A

O. J. Glembocki, 1988). For example, thermal modulation produces a first derivative spectrum while the electro-modulation generates a third derivative spectrum. However, the same form of equation (3.15) can be used for all the Lorentzian type line shapes with the only adjustment of n , which represents the proper critical point dimensions. The appropriate choices of n are listed in Table I (F. H. Pollak and O. Glembocki, 1988).

3.3 Screened 2D-Exciton

In the presence of a sufficiently dense 2DEG (or 2D plasma) the intersubband absorption function will be a broadened two dimensional density of states modified by a Fermi level filling factor. The imaginary part of dielectric function can be thus expressed as:

$$\begin{aligned} \epsilon_2 &= I(1-f_e) \text{Im}(\epsilon^{2D}) \\ f_e^{-1} &= 1 + \exp \left[\frac{\frac{m_h^*}{m_e^* + m_h^*} (E - E_x) - \Delta E_F^x}{k_B T} \right] \\ \epsilon^{2D} &= \ln(E - E_x + i\Gamma) \end{aligned} \quad (3.16)$$

where all the parameters have the same meanings as the unscreened exciton case except the extra parameter ΔE_F^x , which is the energy difference between the Fermi level and the position of the conduction subband involved in the transition E_x .

By using the Kramers-Kronig relation the ϵ_1 can be obtained. All the line shape functions are then obtained by taking appropriate derivative operations.

Chapter 4. Theoretical Calculation Methods

4.1 Hamiltonian in Zinc-blende Type Materials

4.1.1 *k.p* Method in Bulk Material

In order to obtain the electronic band structure of a material without any external perturbations, we need to solve the Schrodinger equation:

$$H|\varphi_k^i\rangle = E^i(k)|\varphi_k^i\rangle \quad (4.1)$$

This is certainly universal to all the systems. The distinctive long range periodicity of the solid state material yields the Bloch wavefunction, which can be expressed as a plane wave $|f_k\rangle$ modulated by a periodic function $|u_k\rangle$.

$$|\varphi_k^i\rangle = |u_k\rangle |f_k\rangle \quad (4.2)$$

where the first term has all the symmetries of the crystal, i.e.,

$$u_k^i(r+R) = u_k^i(r) \quad (4.3)$$

and the second term is the plane wave with wave vector $\mathbf{k}$:

$$f_k(r) = e^{ikr} \quad (4.4)$$

The Hamiltonian can thus be written down as:

$$H = \frac{P^2}{2m_e} + V = \frac{(P_u + P_f)^2}{2m_e} + V \quad (4.5)$$

where the momentum operator $\mathbf{P}$ is broken into two momentum operators $\mathbf{P}_u$ and $\mathbf{P}_f$, which acting only on the periodic part $|u_k\rangle$ and plane wave part $|f_k\rangle$ of the Bloch wavefunction, respectively.

$$\begin{aligned} P_u |u_k\rangle &\neq 0 & P_u |f_k\rangle &= 0 \\ P_f |u_k\rangle &= 0 & P_f |f_k\rangle &= \hbar \vec{k} \end{aligned} \quad (4.6)$$

The problem is thus in principle defined and ready to be solved. The most difficult part in Eq.(4.5) is the lattice potential V . Using $k.p$ perturbation theory, suppose we know the solutions at Γ point ($k=0$),

$$H_0 |u_0^i\rangle = \left(\frac{P_u^2}{2m_e} + V \right) |u_0^i\rangle = \epsilon_0^i |u_0^i\rangle \quad (4.7)$$

Using the completeness property of the wavefunction basis $|u_0^i\rangle$, we can express the lattice potential V in terms of the knowledge at Γ point. Therefore, the Hamiltonian can be expressed as,

$$\begin{aligned} H &= \frac{(P_u + P_f)^2}{2m_e} + V \sum_i |u_0^i\rangle \langle u_0^i| \\ &= \frac{(P_u + P_f)^2}{2m_e} + \sum_i \left(\epsilon_0^i - \frac{P_u^2}{2m_e} \right) |u_0^i\rangle \langle u_0^i| \\ &= \sum_i \epsilon_0^i |u_0^i\rangle \langle u_0^i| + \frac{P_u P_f}{m_e} + \frac{P_f^2}{2m_e} \\ &= H_0 + H_1 + H_2 \end{aligned} \quad (4.8)$$

There is no approximation so far. One can in principle solve the problem in the basis $|u_0\rangle$ if the matrix elements can be evaluated, i.e.,

$$|u_k\rangle |f_k\rangle = (\sum_j a_{ij} |u_0^j\rangle) |f_k\rangle \quad (4.9)$$

In the bulk case, the operator $\mathbf{P}_f$ is very easy. One simply substitute $\hbar\mathbf{k}$ with every occurrence of $\mathbf{P}_f$ operator, and throw away the common plane wave-function $|f_k\rangle$. The matrix element of $\langle u_0^j | \mathbf{P}_u | u_0^i \rangle$ is the difficult part. Although they can be evaluated from various first principle calculations, these matrix elements can be deduced more accurately from the various experimental critical point values. The amount of necessary matrix elements can be significantly reduced by considering the material symmetry properties. This simple yet accurate approach has been widely used in the semiconductor electronic band structure calculations.

4.1.2 Zinc-blende Type Material near E_0

For practical treatment, one need to make some assumptions in order to reduce the size of Hamiltonian matrix, or number of electronic bands. Only a few bands are needed if the interested region is within the vicinity of Γ point (small k), because the perturbation terms H_1 and H_2 increase with the increasing k value. In this work, we are dealing with the GaAs (or GaAs-alike) Zinc-blende type material. Most attentions have been paid to the features arisen from the E_0 . This requires to include the lowest Γ_1 conduction band and highest three Γ_{15} valence bands (with double Kramer's degeneracy).

We will use the following wavefunction notations for these electronic bands:

$$\begin{aligned}
 |c\rangle_{\pm} &= |S\rangle_{\xi_{\pm}} \\
 |\frac{3}{2}, \pm\frac{1}{2}\rangle &= \frac{1}{\sqrt{6}}(X \pm iY)\xi_{\mp} - \sqrt{\frac{2}{3}}Z\xi_{\pm} \\
 |\frac{3}{2}, \pm\frac{3}{2}\rangle &= \frac{1}{\sqrt{2}}(X \pm iY)\xi_{\pm} \\
 |\frac{1}{2}, \pm\frac{1}{2}\rangle &= \pm\frac{1}{\sqrt{3}}(X \pm iY)\xi_{\mp} \pm \frac{1}{\sqrt{3}}Z\xi_{\pm}
 \end{aligned} \tag{4.10}$$

where ξ_+ (ξ_-) denotes the spin up (down). The conduction band $|c\rangle$ has the S (Γ_1) symmetry, and the three P (Γ_{15}) symmetry valence bands are divided into a J=3/2 doublet and a J=1/2 singlet due to spin-orbit interaction (see Fig. 6).

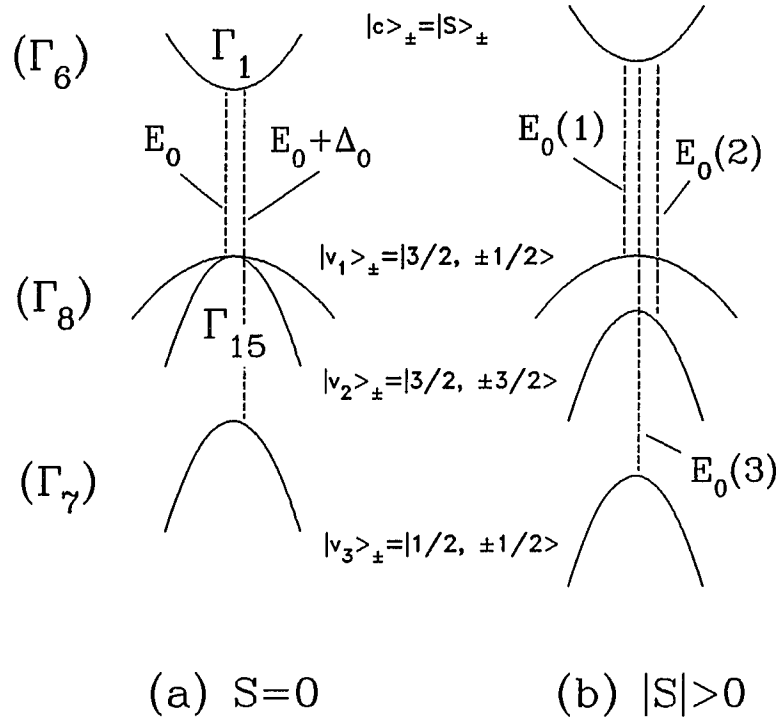


FIG. 6 Schematic band diagram near Γ point for zinc-blende type materials.

The Hamiltonian matrix element with up to second order perturbation under these eight basis functions (including Kramers degeneracy) can be expressed as (E. O. Kane, 1966):

$$\begin{aligned}
 [H] &= [H_0+H_2] + [H_1^{(1)}] + [H_1^{(2)}] \\
 \langle j|H|i\rangle &= (\epsilon_0^i + \frac{\hbar^2 k^2}{2m_e})\delta_{ij} + \langle j|H_1|i\rangle + \sum_n' \frac{\langle j|H_1|n\rangle \langle n|H_1|i\rangle}{\epsilon_0^i - \epsilon_n^i}
 \end{aligned} \quad (4.11)$$

where the first term is diagonalized, the second term has no coupling among conduction or valence bands themselves due to Γ_{15} symmetry of $k.p$ operator H_1 , and the third term describes the interaction through second order perturbations with the rest electronic bands which are not included explicitly in our basis subset.

At $k_x=k_y=0$, the total 8×8 Hamiltonian is decoupled into two identical 4×4 matrix (F. H. Pollak, 1990):

$$[H] = \begin{bmatrix}
 |c\rangle_{\pm} & |\frac{3}{2}, \pm\frac{1}{2}\rangle & |\frac{3}{2}, \pm\frac{3}{2}\rangle & |\frac{1}{2}, \pm\frac{1}{2}\rangle \\
 E_0 + (1+D_c')\frac{\hbar^2 k_z^2}{2m_0} & -i\frac{P\hbar k_z}{\sqrt{3m_0}} & 0 & i\frac{P\hbar k_z}{\sqrt{6m_0}} \\
 i\frac{P\hbar k_z}{\sqrt{3m_0}} & (1+A'+B')\frac{\hbar^2 k_z^2}{2m_0} & 0 & \frac{B'\hbar^2 k_z^2}{\sqrt{2}m_0} \\
 0 & 0 & (1+A'-B')\frac{\hbar^2 k_z^2}{2m_0} & 0 \\
 -i\frac{P\hbar k_z}{\sqrt{6m_0}} & \frac{B'\hbar^2 k_z^2}{\sqrt{2}m_0} & 0 & -\Delta_0 + (1+A')\frac{\hbar^2 k_z^2}{2m_0}
 \end{bmatrix} \quad (4.12)$$

where E_0 , Δ_0 , $\hbar$ and m_0 are the fundamental band gap, spin-orbit split, Plank constant, and free electron mass, respectively. Four parameters are involved, they are first order process P due to $H_1^{(1)}$, and second order processes A' , B' , and D'_c due to $H_1^{(2)}$. The explicite expressions of these parameters are listed by F. H. Pollak (1990).

The effects of various external perturbations can be included in this presentation simply by adding in the appropriate Hamiltonian in the same set of basis functions.

$$H_{total} = H_{k,p} + H_\epsilon + eFz + \dots \dots \quad (4.13)$$

4.1.3 Uniaxial Stress Effects in Bulk Materials

For example, the strain deformation ϵ_{ij} is defined as,

$$\begin{aligned} r_i^\epsilon &= a_{ij} r_j \\ a_{ij} &= \delta_{ij} + \epsilon_{ij} \end{aligned} \quad (4.14)$$

The strain Hamiltonian can be written down as,

$$\begin{aligned} \therefore V_\epsilon(r_i) &= V(a_{ij}^{-1} r_j) = V(r_i - \epsilon_{ij} r_j) = V(r_i) - \epsilon_{ij} r_j \frac{\partial V}{\partial r_i} \\ \therefore H_\epsilon &= V_\epsilon(r_i) - V(r_i) = -\epsilon_{ij} r_i \frac{\partial V}{\partial r_j} \end{aligned} \quad (4.15)$$

Since the operator H_ϵ has the same symmetry property as the $H_1^{(2)}$ ($\propto P_u^2$), the strain Hamiltonian should have similar behavior as $H_1^{(2)}$. One can show that this symmetry argument results in the same matrix elements to a detailed evaluation based

on the following strain Hamiltonian:

$$\begin{aligned} H_\epsilon^c &= a_c \text{Tr}(\epsilon) \\ H_\epsilon^v &= -a_v \text{Tr}(\epsilon) - b[(L_z^2 - \frac{1}{3}L^2)\epsilon_{zz} + c.p.] - \sqrt{3}d[(L_x L_y + L_y L_x)\epsilon_{xy} + c.p.] \end{aligned} \quad (4.16)$$

where a , b , and d are the deformation potentials corresponding to hydrostatic (O_h), tetragonal (D_{4h}), and trigonal (S_6 , C_{3i}) deformations, respectively, a_c and a_v are the absolute band edge shift of conduction and valence bands, L_i ($i=1,2,3$) is the angular momentum operator of i th component, and $c.p.$ denotes the cyclic permutation.

If $\epsilon_{xz} = \epsilon_{yz} = 0$, which is satisfied in all of our experimental configurations of this work ($S \parallel [001]$, $[100]$, or $[110]$), the 8×8 strain Hamiltonian becomes two decoupled identical 4×4 matrix.

$$[H_\epsilon] = \begin{bmatrix} \delta E_a^c & 0 & 0 & 0 \\ 0 & -(\delta E_a^v - \delta E_b) & -(\delta E_b^1 - i\delta E_d) & \sqrt{2}\delta E_b \\ 0 & -(\delta E_b^1 + i\delta E_d) & -(\delta E_a^v + \delta E_b) & \sqrt{2}(\delta E_b^1 + i\delta E_d) \\ 0 & \sqrt{2}\delta E_b & \sqrt{2}(\delta E_b^1 - i\delta E_d) & -\delta E_a^v \end{bmatrix} \quad (4.17)$$

where δE_a^c , δE_a^v , δE_b , δE_b^1 , and δE_d are defined as:

$$\left\{ \begin{array}{l} \delta E_a^c = a_c(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \\ \delta E_a^v = a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \\ \delta E_b = b[\epsilon_{zz} - \frac{1}{2}(\epsilon_{xx} + \epsilon_{yy})] \\ \delta E_b^1 = \frac{\sqrt{3}}{2}b(\epsilon_{xx} - \epsilon_{yy}) \\ \delta E_d = d\epsilon_{xy} \end{array} \right. \quad (4.18)$$

The strain components due to a stress S along [001] (equivalently [010] and [100]) are $\epsilon_{zz} = S_{11}S$, $\epsilon_{xx} = \epsilon_{yy} = S_{12}S$, and $\epsilon_{xy} = \epsilon_{yz} = \epsilon_{zx} = 0$. The stress dependence of various transitions is:

$$\begin{aligned} E_0(1) &= E_0 + \delta E_H - \delta E_{001} - \frac{2\delta E_{001}^2}{\Delta_0} + O\left(\frac{\delta E_{001}^3}{\Delta_0^2}\right) \\ E_0(2) &= E_0 + \delta E_H + \delta E_{001} \\ E_0(3) &= E_0 + \delta E_H + \frac{2\delta E_{001}^2}{\Delta_0} + O\left(\frac{\delta E_{001}^3}{\Delta_0^2}\right) \end{aligned} \quad (4.19)$$

where $\delta E_H = \delta E_a^c + \delta E_a^v = a(S_{11} + 2S_{12})S$ and $\delta E_{001} = \delta E_b = b(S_{11} - S_{12})S$.

For a stress $S \parallel [110]$, the strain components are $\epsilon_{xx} = \epsilon_{yy} = (S_{11} + S_{12})S/2$, $\epsilon_{zz} = S_{12}S$,

$\epsilon_{xy}=S_{44}S/4$, and $\epsilon_{yz}=\epsilon_{xz}=0$. The stress dependence of the transitions are:

$$\begin{aligned}
 E_0(1) &= E_0 + \delta E_H - \delta E_{110} - \frac{2\delta E_{110}^2}{\Delta_0} - \frac{3\delta E_\delta^2}{32\delta E_{110}} + O\left(\frac{\delta E_{110}^3}{\Delta_0^2}\right) + O\left(\frac{\delta E_\delta^3}{\delta E_{110}^2}\right) \\
 E_0(2) &= E_0 + \delta E_H + \delta E_{110} + \frac{3\delta E_\delta^2}{32\delta E_{110}} - \frac{27\delta E_\delta^2}{32\Delta_0} + O\left(\frac{\delta E_{110}^3}{\Delta_0^2}\right) + O\left(\frac{\delta E_\delta^3}{\delta E_{110}^2}\right) \\
 E_0(3) &= E_0 + \delta E_H + \frac{2\delta E_{110}^2}{\Delta_0} + \frac{27\delta E_\delta^2}{32\Delta_0} + O\left(\frac{\delta E_{110}^3}{\Delta_0^2}\right) + O\left(\frac{\delta E_\delta^3}{\delta E_{110}^2}\right)
 \end{aligned} \quad (4.20)$$

where $\delta E_H = a(S_{11} + 2S_{12})S$, $\delta E_{110} = (\delta E_b + 3\delta E_d)/4$, $\delta E_\delta = \delta E_b - \delta E_d$, with $\delta E_b = b(S_{11} - S_{12})S$,

$$\delta E_d = \frac{dS_{44}S}{2\sqrt{3}}.$$

4.1.4 Envelope Function Approximation in Semiconductor Microstructures

In semiconductor microstructures, the long range periodicity has been changed. We will only examine the layered structures along z directions. In these structures, the disappearance of z direction long range periodicity makes the plane wave function no longer valid for the growth direction, i.e.,

$$\langle r | f_k \rangle = e^{i(k_x x + k_y y)} f(k_z; z) \quad (4.21)$$

here the k_z is either continuous (in SLs) or discrete (in QWs) and the $f(k_z; z)$ is usually called envelope function because it is a even slower varying function than the $|u_k\rangle$.

Therefore, the z component of the operator P_r can not be simply substituted by $\hbar k_z$ and

eliminate the common $|f_k\rangle$ as in the case of bulk materials. Instead its original operator form has to be used and acted onto the envelope functions $|f_k\rangle$.

When the material layers involved are not extremely thin, the Hamiltonian matrix form of Eq. (4.11) is still valid if the material related parameters ϵ_0^i and $P^{ji} = \langle j | P_u | i \rangle$ are taken piecewise corresponding to the material layer and the z component of operator $\mathbf{P}_f$ is kept in its operator form and the $|f_k\rangle$ is in more general form instead of a plane wave along z direction.

In actual calculations, further assumptions are needed. Two widely used assumptions are (a) the rapid varying Bloch wavefunction $|u_0\rangle$ is material independent so that the basis functions on which the Hamiltonian is expressed are common in different layers and (b) in plane momentum k_x and k_y are conserved across different layers so that it can be simplified into a one dimensional problem along the growth (z) direction.

4.1.5 Effective Mass Model

In most situations, we are only interested in the critical points at $k_x=k_y=0$, i.e., Eq. (4.12). Further approximations yield various calculation approaches, each with its own convenience and accuracy. As an example, by taking the H_1 term implicitly, all the coupling among these bands are neglected (W. Kohn, 1957). In this effective mass

(quadratic band) approximation, each band can be evaluated separately. One has several decoupled differential equations. Each of them has the following identical form,

$$-\frac{\hbar^2}{2m^*(z)} \frac{d^2 f(k_z; z)}{dz^2} + \epsilon_0(z) f(k_z; z) = E(k_z) f(k_z; z) \quad (4.22)$$

where the effective mass $m^*(z)$ and band edge $\epsilon_0(z)$ are material varying parameters.

This is a very convenient model. It predicts correctly where the mass non-parabolicity of the band is small. In another word, the result is good for energies which correspond to small k_z on the bulk dispersion curve.

4.1.6 Bastard Model

Another approximation is obtained by taking the $H_1^{(1)}$ terms explicitly while neglecting the second order perturbations of Hamiltonian $H_1^{(2)}$ as well as H_2 (G. Bastard and A. Brum, 1986). This is the so called Bastard model, where the $|v_2\rangle$ band are decoupled, and the conduction band is coupled with the $|v_1\rangle$ band. The nonparabolicity effect due to the $|c\rangle - |v_1\rangle$ coupling is rigorously included. The calculation of the $|v_2\rangle$ band is the same as the effective mass approximation. However, calculations of $|c\rangle$ and $|v_1\rangle$ bands are more complicated since now we have two coupled differential equations. Neglecting $|v_3\rangle$ band in Eq. (4.12), we have the following equations,

$$\begin{aligned}
(E_0 - E)f_c - \frac{P\hbar}{\sqrt{3m_e}} \frac{df_v}{dz} &= 0 \\
-\frac{P\hbar}{\sqrt{3m_e}} \frac{df_c}{dz} - Ef_v &= 0
\end{aligned} \tag{4.23}$$

They can be expressed by two decoupled second order differential equations:

$$\begin{aligned}
\frac{d^2 f_c}{dz^2} + \frac{3m_e E(E - E_0)}{\hbar^2 P^2} f_c &= 0 \\
\frac{d^2 f_v}{dz^2} + \frac{3m_e E(E - E_0)}{\hbar^2 P^2} f_v &= 0
\end{aligned} \tag{4.24}$$

This is formally the same as effective mass model if the energy dependent effective mass is taken as,

$$\begin{aligned}
m_c^* &= \frac{3E}{2P^2} m_e = \frac{3(E_0 + \Delta E_c)}{2P^2} \\
m_{LH}^* &= -\frac{3(E_0 - E)}{2P^2} m_e = -\frac{3(E_0 + \Delta E_{HH})}{2P^2}
\end{aligned} \tag{4.25}$$

where ΔE_c and ΔE_{HH} are the carrier kinetic energies due to quantum confinement of the conduction band and HH valence band, respectively. These expressions show that only the $|c\rangle - |v_1\rangle$ coupling is considered in the effective mass origin.

The difference between this effective mass expression and the more accurate one (F. H. Pollak, 1990) at Γ point is negligible when $P^2 \gg 0$ (such as GaAs) so that the

results will be similar to the effective mass calculations at low energy. However, this model has reported to give improved results for high energy transitions due to its mass correction scheme.

More rigorous approaches have also been proposed by other workers such as Potz *et al* (1985) and Smith and Mailhot (1986). We will not discuss them here, since the two simple models are already enough for most practical situations where the $k.p$ Hamiltonian is still valid. We will raise the example of QWs.

4.1.7 QW Structure

In SQWs due to the uncertainty principle, the ground state can no longer be at $k_z=0$ because of the confinement $\Delta z \leq L_z$. The new electronic dispersion curve along z direction becomes now a series of discrete levels, and the quantum number k_z is conveniently replaced by a new discrete quantum number n .

Using the effective mass model (solid circles) and the Bastard model (squares), various symmetry-allowed quantum transitions are calculated as a function of L_z in Fig. 7 for GaAs/Al_{0.3}Ga_{0.7}As SQWs. The dashed lines at 440meV is the energy gap difference of $E_0(\text{AlGaAs})-E_0(\text{GaAs})$. It can be seen that when the L_z increases (a) the ground state energy is approaching the bulk $E_0(\text{GaAs})$ since k_z approaches zero due to increasing uncertainty of Δz , (b) more and more transitions are possible, and (c) the distribution of all the transitions approaches the dispersion curve of a bulk material, i.e.,

a quadratic one ($E_n \propto n^2 \propto k_z^2$).

For the transitions with less than 200 meV confinement energy, the effective mass approximation gives very good results. The nonparabolicity effect is noticeable only when confinement energy is bigger than 200 meV, which is the case for either higher order transitions or in narrow QWs. Therefore, we will use the effective mass model later on for its simplicity.

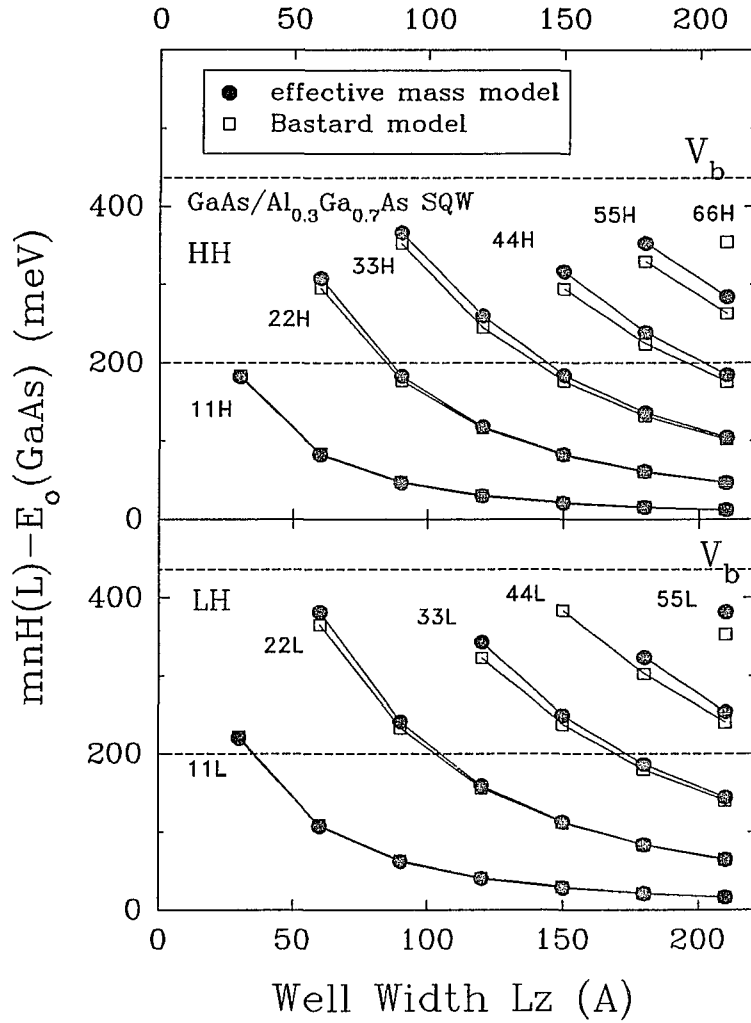


FIG. 7 Quantum transitions in GaAs/Al_{0.3}Ga_{0.7}As QWs calculated by the effective mass (solid lines) and Bastard (dashed lines) models.

4.2 Numerical Self-consistent Calculation of HEMT Structures

In the presence of a dense carrier concentration such as the 2DEG in HEMT structures, the free carriers can change the band profile significantly due to direct

Coulomb interaction as well as exchange Coulomb interaction (band gap renormalization). The Schrodinger and Poisson equations will form a coupled system, which is formally similar to a one dimensional atomic Hartree-Fock self-consistent field problem. Using the simple effective mass approximation, the single electron Schrodinger equation for the conduction band can be expressed as:

$$\left[\frac{P_f^2}{2m^*} + V_b(z) + V_{sc}(z) + V_{xc}(z) + V_{lm}(z) \right] f_n(z) = E_n f_n(z) \quad (4.26)$$

where $V_b(z)$ is the heterostructure conduction band discontinuity due to H_0 term, $V_{sc}(z)$ is the static Coulomb potential which is determined by the Poisson equation (see section 4.2.2).

V_{xc} is the non-local exchange potential due to Pauli principle. It is usually approximated by the local density approximations as a localized potential. One such example is:

$$\begin{aligned} a_s &= \frac{4\pi\epsilon_0\kappa\hbar^2}{me^2} \quad r_s = \left[\frac{4}{3}\pi a_s^3 n(z) \right]^{-\frac{1}{3}} \quad x = \frac{r_s}{21} \\ a &= \left[\frac{4}{9\pi} \right]^{\frac{1}{3}} \quad R_y = \frac{e}{8\pi\epsilon_0\kappa a_s} \\ V_{xc}(z) &= - \left[1 + 0.7734x \ln\left(1 + \frac{1}{x}\right) \right] \left(\frac{1}{\pi a r_s} \right) R_y \end{aligned} \quad (4.27)$$

And V_{IM} is contribution from the image charges across the interface due to different dielectric constants κ of the different material layers. For GaAs/AlGaAs material systems it is believed to be very small since the κ difference is very small.

The nature of this problem makes it impossible to achieve an analytical solution. Its answer can only be obtained numerically. This problem can be broken down into a numerical Schrodinger equation solver, a numerical Poisson equation solver, and a self-consistent solution finder. Each will be discussed separately here.

4.2.1 Numerical Schrodinger Equation Solver

The Schrodinger equation solver requires a numerical solver to a second order differential equation of the following form,

$$-\frac{1}{a(z)} \frac{d^2 f_n(z)}{dz^2} + b(z) f_n(z) = c_n f_n(z) \quad (4.28)$$

where the $a(z)$ and $b(z)$ are given functions of z , the eigen-problem is attempted for the n th solution with the vanishing boundary conditions $f_n(z)=0$ at either end. The quantum number n of eigenvalue c_n and eigenfunction $f_n(z)$ can be determined from the number of nodes of $f_n(z)$.

By substituting the differential operators with appropriate finite difference operators, the solution to this eigen problem can be attempted numerically. Two most

common numerical approaches to the two point boundary value eigen problems are the shooting and relaxation methods (W. H. Press *et al*, 1986). Either has its advantages and disadvantages. Our implementation is a hybridation of both in order to combine their advantages. At first round where we have no knowledge about the system, the shooting method is used to find the solution. Later on the relaxation method is used during the self-consistent iterations. There are several advantages of iterative relaxation method such as (a) the faster speed by utilizing the former knowledge about the system and (b) better precision in personal computer environment because of no round-off error accumulation mechanism which is intrinsic in shooting method.

4.2.2 Numerical Poisson Equation Solver

The objective of this program module is to determine the appropriate Fermi energy level, charge distributions, and thus Coulomb static potential based on the input of electronic wavefunctions.

The Fermi level E_f is determined from the charge neutrality requirement:

$$\int_{-\infty}^{\infty} n_{total}(E_f; z) dz = 0 \quad (4.29)$$

with

$$n_{total}(E_f; z) = \sum_i n_i(E_f) |f_i(z)|^2 - p(E_f; z) - N_D^+(E_f; z) + N_A^-(E_f; z) \quad (4.30)$$

where the four terms on the right side of the equation represent the contributions from

the free electrons, free holes, ionized donors, and ionized acceptors, respectively. For a HEMT structure, they are:

$$\left\{ \begin{array}{l} n_i(E_f) = \frac{k_B T}{\pi \hbar^2} \ln[1 + \exp(\frac{E_f - E_i}{k_B T})] \\ p(E_f; z) \approx 0 \\ N_D^+(E_f; z) = \frac{N_D}{\frac{1}{2} + \exp(\frac{E_D(z) - E_f}{k_B T})} \\ N_A^-(E_f; z) = \frac{N_A}{\frac{1}{2} + \exp(\frac{E_f - E_A(z)}{k_B T})} \approx 0 \end{array} \right. \quad (4.31)$$

where E_i is the i th electron sublevel determined by the Schrodinger equation, E_D , E_A , and E_f are the donor level, acceptor level, and Fermi level, respectively, k_B is the Boltzmann constant, and $\hbar$ is the Plank constant. The expression of the n_i is deduced from the step-like 2D density of states distribution. For 2DEG HEMT structures, the contributions from the free holes and acceptors can usually be neglected.

Once the charge distribution $n_{total}(z)$ is known, the static Coulomb potential can be determined from the following Poisson equation,

$$\frac{d^2 V_{sc}(z)}{dz^2} = - \frac{e}{\epsilon_0 \kappa(z)} n_{total}(z) \quad (4.32)$$

4.2.3 Self-consistent Solution Algorithm

The flowchart of our self-consistent solution iteration algorithm is shown in Fig.

8. The initial potential and wave-functions are either from approximated analytical solutions or from earlier calculation results of similar structures. The Schrodinger and Poisson solvers are invoked in turn to converge to a final self-consistent solution. The convergence behavior and speed requirement of an algorithm are two competing considerations. We have adopted the convergence algorithm proposed by F. Stern (1970), where in the i th iteration round only a portion (w_i) of calculated difference of the solution is accepted,

$$f^{(i+1)} = f^{(i)} + w_i(f^{calc} - f^{(i)}) \quad (4.33)$$

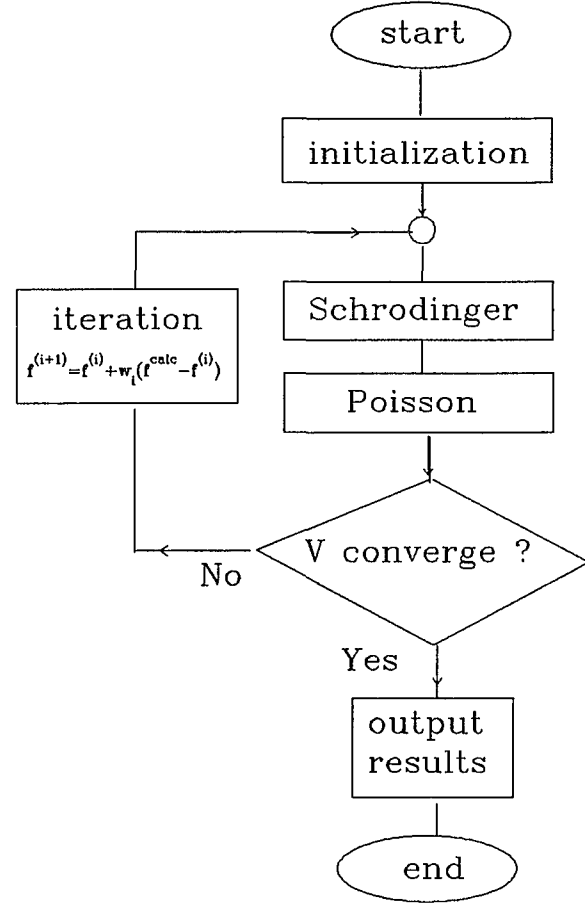


FIG. 8 Flowchart of the self-consistent solution finder.

The factor w_i , which is independent of z , is usually taken between 0 and 1. A small value gives smooth but slower convergence, while a value close to 1 gives rapid convergence in some cases, but leads to diverging results in others. We have used several fixed w_i round and then the extrapolated-convergence-factor method as proposed

by F. Strern (1970). This dynamical w_i factor gives satisfactory performance since it can optimize the convergence speed in real time while safeguard the possible divergence crisis. The iteration stops when the difference between the calculated and input potentials is smaller than a preset value.

4.3 QW and CDQW under Electric Field

We are only dealing with the electric field along the growth (z) direction. This electric field alone is relatively simple. The field perturbation is already diagonalized in our matrix representation. If we use the effective mass (parabolic band) approximation, all the four bands remain decoupled. The situation will be similar for each of these bands. Since SQW is an extremal case of CDQWs when either the barrier between two wells is zero or one well has zero width, we will concentrate here on the CDQW structures.

We have tried several methods in calculating the energy levels in a CDQW. The first method we tried is the numerical shooting and relaxation method modified from the Schrodinger equation solver of the previous section similar to a recent report of W. L. Bloss (1990). This method yields satisfactory results at low fields but poorer at high fields. The convergence boundary condition in the barrier region, the basic requirement of a *true* confined state, is not strictly valid when the electric field is applied. The higher the field is, the closer we have to move the cut-off points to the CDQW region, and poorer the results will be. In fact if the field is high enough, one no longer be able to

set the proper cut-off position since there is not a thick enough tunneling barrier so that the wavefunctions can decay to a negligible magnitude. Another method has been suggested by J. Lee *et al* (1989), where the numerical differentiation is avoided by using exact solutions of Airy functions, and the cut-off points are chosen at the physical boundaries of thick barrier layers of actual device structures. While it is arguable to set wavefunction to zero at those points, the influence to the CDQW transition energies by the distance change between the artificial infinite barrier and CDQW region is much larger than one might expect at first glance. There will exist some states at triangle well region formed by the tilted lower barrier and the artificial infinite barrier. As the field increases, these levels lower down when the potential profile tilts more. Whenever they cross the resonance positions in CDQW region, the anticrossing may occur. This can be serious enough to create a series of discontinuous points on the field dependence of CDQW levels. This irregular phenomenon is physically unrealistic. It has been a serious problem to us for a while before we realize that it is due to the intrinsic origin of this approach instead of the detailed implementations. This situation was also observed on the calculation results reported by J. Lee *et al* (1990). Therefore, the confined state approaches are not proper choices here. In order to have a method which is capable of dealing with high electric field, we have extended the resonance method of E. J. Austin and M. Jaros (1985). At low fields our calculations show that all the methods agree with each other fairly well, while at high field only the resonance method yields satisfactory smooth varying results which agree with experimental observations. Besides the energy positions can be extracted with more physical sense, the density-of-

state curve vividly shows more information, such as the field induced broadening, the coupling behavior, and the level crossing resonance (e.g. see $2h$ and $3h$ levels in Fig. 11).

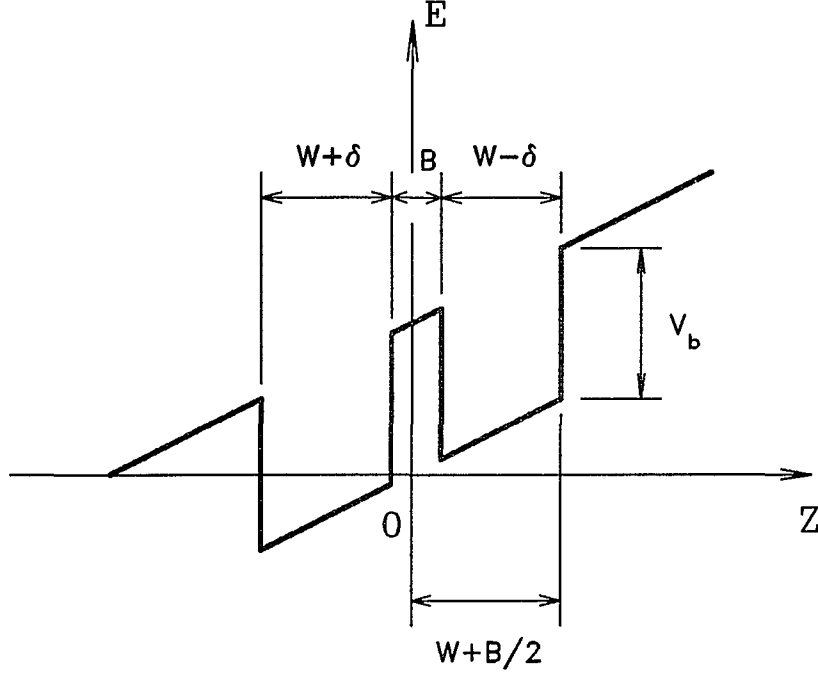


FIG. 9 Schematic band diagram of a CDQW under electric field.

Shown in Fig. 9 is a schematic diagram for one band (conduction or HH or LH bands) of a CDQW structure. Two quantum wells of well width $W+\delta$ and $W-\delta$ are coupled through a barrier of thickness B . The barrier height is V_b . The origin is chosen at the mid point of CDQW region. The Hamiltonian of this system can be expressed as:

$$-\frac{\hbar^2}{2m_z^*} \frac{d^2 f(z)}{dz^2} + V_z f(z) + eFz f(z) = E f(z) \quad (4.34)$$

where effective mass m_z^* and V_z are material and system dependent,

$$\begin{cases} m_z^* = m_b^* & V_z = V_b & (z \in \text{barrier}) \\ m_z^* = m_w^* & V_z = 0 & (z \in \text{well}) \end{cases} \quad (4.35)$$

By taking the following variable transformation,

$$\xi = \left[\frac{2m_z eF}{\hbar^2} \right]^{\frac{1}{3}} \times \left[z - \frac{E - V_z}{eF} \right] \quad (4.36)$$

the Schrodinger equation can be simplified as:

$$\frac{d^2 f(\xi)}{d\xi^2} - \xi f(\xi) = 0 \quad (4.37)$$

Its solutions are the Airy functions $Ai(\xi)$ and $Bi(\xi)$. Therefore, the wavefunction can be expressed as:

$$f(z) = \begin{cases} A_1 Ai(\xi) + B_1 Bi(\xi) & z \in (-\infty, -W - \frac{B}{2}) \\ A_2 Ai(\xi) + B_2 Bi(\xi) & z \in [-W - \frac{B}{2}, -\frac{B}{2} + \delta) \\ A_3 Ai(\xi) + B_3 Bi(\xi) & z \in [-\frac{B}{2} + \delta, \frac{B}{2} + \delta) \\ A_4 Ai(\xi) + B_4 Bi(\xi) & z \in [\frac{B}{2} + \delta, W + \frac{B}{2}) \\ A_5 Ai(\xi) & z \in [W + \frac{B}{2}, \infty) \end{cases} \quad (4.38)$$

here $B_5 = 0$ because of the wavefunction convergence requirement at $z \rightarrow \infty$.

Using boundary conditions of the effective mass approximation at four interfaces, all the wavefunction coefficients can be expressed in terms of A_5 . In particular, the information of the CDQW resonant behavior is implied inside the ratios of A_1/A_5 and B_1/A_5 . In strict sense no bound states will exist in the presence of an electric field. Two approaches are suggested to find the resonance energies (quasi bound states).

The phase angle and the Breit-Wigner parameterization are defined as (E. J. Austin and M. Jaros, 1985):

$$\tan\phi = \frac{B_1}{A_1} = \frac{\Gamma}{2(E-E_0)} \quad (4.39)$$

where E_0 is the resonance energy, Γ is the broadening parameter. Thus, from the energy dependence of the phase angle ϕ , the E_0 and Γ can be deduced. We have $A_1=0$ when $E=E_0$. At low field limit when $A_1=0$, this energy position is exactly a bound state since the wavefunction in the barrier region becomes:

$$\begin{aligned} \lim_{z \rightarrow -\infty} f(z) &= \lim_{z \rightarrow -\infty} B_1 Bi(\xi) \rightarrow e^{+|\kappa|z} \\ \lim_{z \rightarrow +\infty} f(z) &= \lim_{z \rightarrow +\infty} A_5 Ai(\xi) \rightarrow e^{-|\kappa|z} \end{aligned} \quad (4.40)$$

The second approach is by examining the difference between the CDQW and the one with the CDQW structure removed. The change of the density of states due to the CDQW structure is defined by (E. J. Austin and M. Jaros, 1985):

$$\Delta\rho = \frac{1}{\pi} \frac{d\phi}{dE} \quad (4.41)$$

The maximum change (peak position) of $\Delta\rho$ is denoted as E_M , which is more appropriate for the optical properties as suggested by Austin and Jaros (1985) especially at high electric field where the E_0 resonance vanishes.

As an example we show the calculations on a GaAs/Al_{0.3}Ga_{0.7}As CDQW structure with $W=60\text{\AA}$, $B=22\text{\AA}$, and $\delta=0$, which is the sample configuration used in our experiment as discussed in section 6.3.2.

The calculated phase angle $\phi(E)$ and the corresponding $\Delta\rho(E)$ of the conduction band are shown in Fig. 10 for an electric field of 50 kV/cm. Above 0.25 eV, the above barrier resonances are observed. These so-called quasi-bound states have been reported experimentally, but they are not our interests in this work. The $\Delta\rho(E)$ curve shows three peaks E_M-1e , E_M-2e , and E_M-3e , which originate from the CDQW region. The $1e$ and $2e$ features can match exactly with the features E_0-1e and E_0-2e of the $\phi(E)$ spectrum as deduced from the condition of $\phi=(n-1/2)\pi$, or $\tan\phi=\infty$. However, the feature $3e$ can not find its correspondance in the $\phi(E)$ spectrum, since the dashed line of $\phi=(3-1/2)\pi$ will not meet with the $\phi(E)$ curve at this field. In another word, no E_0-3e solution exists for $\phi(E)$. At $F=0$, there are two electronic levels in two wells. The resonance coupling between the first levels produces the $1e$ and $2e$ levels, while the resonance coupling of the second level generates only one bound state $3e$ merely inside the CDQW region since the would-be " $4e$ " level is above the barrier by the coupling repulsion. Because the $3e$ is so close to the edge, it is a vonerable feature which can be easily destroyed by an

electric field. The $\phi(E)$ curve does show the third resonance near the edge at small fields, which suddenly disappears near $F=50$ kV/cm when $\phi(E)$ curve loses contact with $\phi=(3-\frac{1}{2})\pi$ line. A better picture is given by the $\Delta\rho(E)$, where the $3e$ resonance can find its twin image $4e$ above the barrier at $F=0$ and the field induced changes are in a smooth style, i.e., its resonance peak broadens more quickly with the application of an electric field than the deep levels of $1e$ and $2e$.

However, it does not vanish abruptly. This suggests that a weaker and broader $3e$ resonance should still be observed at this field instead of zero oscillator strength by the E_0 picture. This is indeed the experimental observations in section 6.3.2. Thus, there are many advantages of using the E_M of $\Delta\rho(E)$ picture.

The calculated $\Delta\rho$ of conduction band and two valence bands (HH and LH) are shown in Fig. 11 for the electric field range $10 \text{ kV/cm} < F < 200 \text{ kV/cm}$ with an

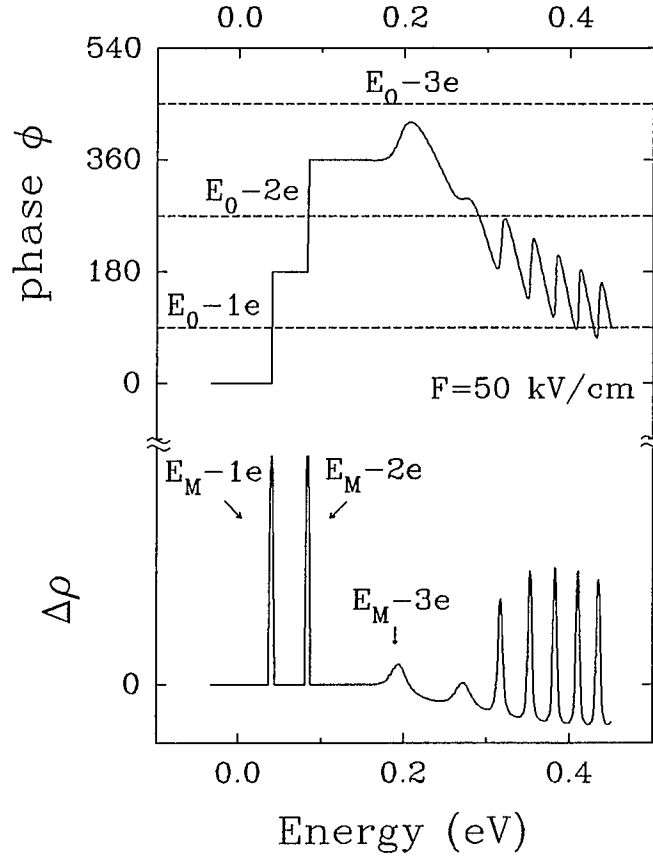


FIG. 10 Calculated phase $\phi(E)$ and $\Delta\rho(E)$ of the conduction band of a GaAs/Al_{0.3}Ga_{0.7}As CDQW structure ($W=60\text{\AA}$, $B=22\text{\AA}$, and $\delta=0$) at $F=50\text{kV/cm}$.

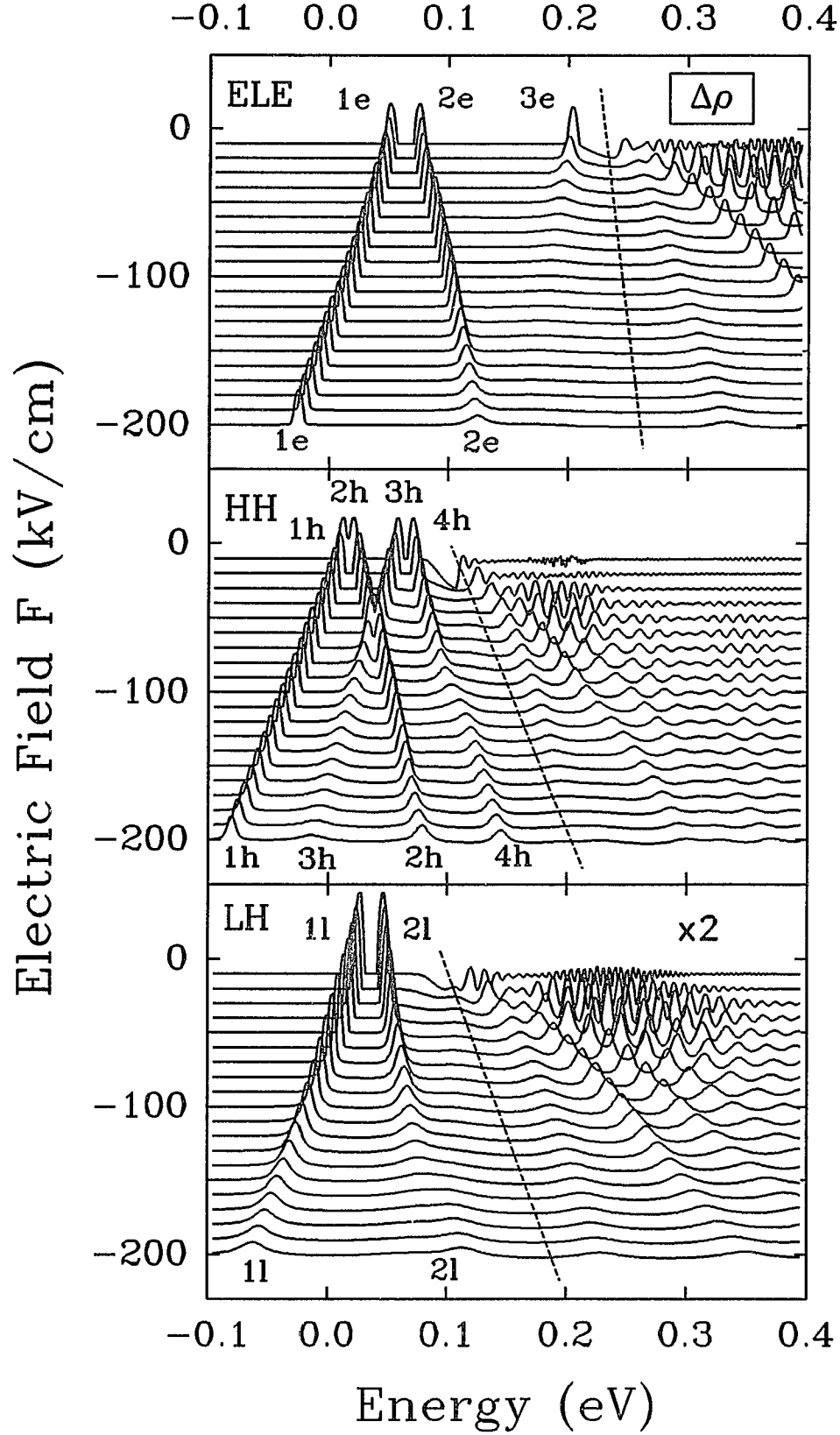


FIG. 11 $\Delta\rho$ of a GaAs/ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ CDQW structure ($W=60\text{\AA}$, $B=22\text{\AA}$, and $\delta=0$) for the electric fields from $10\text{ kV}/\text{cm}$ to $200\text{ kV}/\text{cm}$ in the step of $10\text{ kV}/\text{cm}$.

incremental step 10 kV/cm. The dashed lines are drawn as guide lines between "bound" and "quasi-bound" states. The sharp resonance features from the CDQW regions are evident below these guide lines. The conduction band has three bound states at flatband condition. The twin image of the $3e$ level ($4e$) can be seen above the barrier as a broader resonance. The $1e$ ($2e$) undergoes a redshift (blueshift) due to the electric field. The $3e$ is also redshifted while has much more significant field induced broadening. The HH shows four very sharp resonances at $F=10$ kV/cm, which originates from the resonance coupling between the pair of two HH states in each QW. As the electric field increases, the $1h$ and $3h$ states move towards the lower energy side, while the $2h$ and $4h$ towards the higher energy side similar to the conduction band. The resonance coupling (anti-crossing) of the $2h$ and $3h$ states can be seen near 60 kV/cm. The LH has only two features because of the lighter effective mass. The field induced broadening is much larger than the conduction and HH bands.

The optical transition energies can be obtained by summing up the results of the conduction and valence bands as well as the band gap of the well material. Since optical experiments usually probes exciton features at low field region, the binding energy also needs to be taken into account. In order to estimate the exciton binding energies under different electric fields, we adopted the simple approximation scheme proposed by J. Lee *et al* (1989). The average separation between the electron and hole pairs along the z direction is estimated from their envelope functions. The exciton binding energy is then calculated based on a variational method. In the real calculation, we use the wavefunc-

tions at E_0 instead of E_M , because it usually has better convergence behavior near the CDQW region and the E_0 agrees with the E_M position very well at low fields. In fact it can be shown that both the E_M and E_0 converge to the very same discrete levels of Kronig-Penny model when F goes to zero. However, for $F \geq 100$ kV/cm, this condition is no longer valid since the E_0 gradually moves away from the E_M and vanishes, e.g., $3e$ level as we discussed early. We then take the E_M positions and treat the binding energy as negligible.

4.4 QW under In-plane Uniaxial Stress

The coupling between QWs can happen not only in the real space as we discussed in the previous section, but also across the different electronic bands. For example, an in-plane uniaxial stress produces the coupling between HH and LH bands even at $k_x=k_y=0$. Using the effective mass approximation of $k.p$ Hamiltonian and the strain Hamiltonian, the conduction band is decoupled from the valence bands and can be solved by simple effective mass model. However, the valence bands become more complicated due to stress induced mixing. It is mathematically the same problem as seeking the in-plane dispersion curves for $k_x, k_y \neq 0$. By including the $|\nu_3\rangle$ implicitly, we have the following coupled differential equations system:

$$\begin{bmatrix} H_{11} - \frac{\hbar^2}{2m_1^*} \frac{d^2}{dz^2} & H_{12} \\ H_{12}^* & H_{22} - \frac{\hbar^2}{2m_2^*} \frac{d^2}{dz^2} \end{bmatrix} \begin{bmatrix} f_1(z) \\ f_2(z) \end{bmatrix} = E \begin{bmatrix} f_1(z) \\ f_2(z) \end{bmatrix} \quad (4.42)$$

where H_{11} , H_{12} , and H_{22} include contributions of both $k.p$ and strains [see Eq. (4.12) and (4.17)].

This coupling may again cause difficulties to the bound state approaches. As schematically illustrated in Fig. 12, the bound state E_x in level 2 can be destroyed by a tiny coupling to level 1 which will act as an escaping channel. Because this tunneling is likely to exist in real situations, bound states is always unrealistic in a strict sense. It only makes sense when the lifetime has been considered. Thus, instead of a bound state calculation to this coupled two level system, we need a resonance approach similar to that we used in the previous section for the structures under electric field.

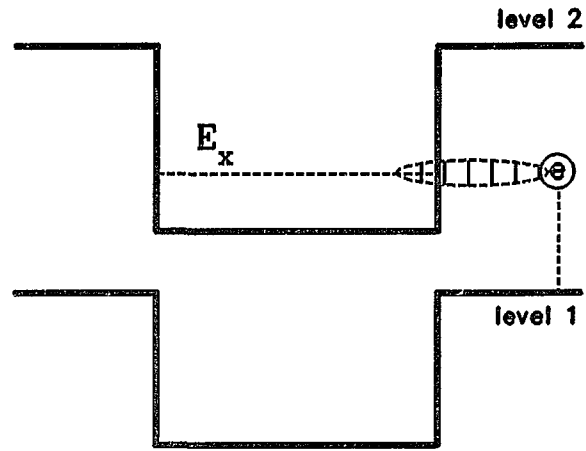


FIG. 12 Schematic potential diagram of a two level quantum well system.

Since the picture of a carrier travelling through several material layers of different V is similar to the situation when a photon travels through several optical films of different n , we have developed a method following the idea of optical matrix approach on a multi-layered film system. The characteristics of the system can be obtained as a product of a series of interface and propagating matrixes. This method has several

advantages such as that (a) it is easy to extend to more complex structures simply by matrix multiplications, (b) it is easy to extend to 3,4 ... higher order coupling systems, (c) resonance (quasi-bound) states are included, and (d) the coupling strength is reflected on off-diagonal elements of the system response matrix. This is the first such theoretical approach to our knowledge which is transplanted from the response matrix of optical multi-films. It is relatively simple to implement and expand to more complicated systems (either complicated profile along z direction or more coupling bands involved), while the physical meaning is quite clear.

A *transfer matrix* algorithm for the calculation of band structures has been proposed by L. R. Ram-Mohan *et al* (1988). It has been shown to yield accurate energy values. Their method is closely related to ours in using the matrix approach. However, these two methods are different in many respects. Our choice of the wavefunction basis in constructing the matrix is more natural by utilizing the idea of propagating plane waves. An implementation transplanted from optics to obtain the matrix is very simple and with clear physical meanings. And a dynamical particle picture can be used to help understand the physical process during each step of the detailed theoretical implementations. Unlike the *transfer matrix* algorithm, each element of our system response matrix represents a physical process, either a transfer channel or a cross link, etc. Also other matrices such as that of the transferring and backscattering (of the normal-mode plane waves) can also be evaluated so that the eigen problem can be simplified. For example, the resonance peaks of the transferring spectra in our approach are very easy to obtain,

while one still has to solve a complicated eigen problem in the *transfer matrix* approach (Ram-Mohan *et al*, 1988). In general, our approach is more simple and relates to a more vivid physical picture.

In order to understand a coupling situation, the usual potential well picture doesn't help very much. We have to choose a better view point. We will use a dynamical picture, which relates to the wave vector $q=k_z$. Let's start with a simple QW structure.

4.4.1 Matrix Method in QW Structure

Shown in Fig. 13(a) is the conventional picture of potential profile of a SQW and the confined ground state wavefunction which consists of two propagating plane waves with wave vector q and $-q$. An equivalent

dynamical picture is

shown in Fig. 13(b), where all the knowledge of the layer is implied in the $q(E)$. Given an E , one has the $q(E)$ so that $f(q)=\exp(\pm iqz)$. We see that the second picture is very similar to the light

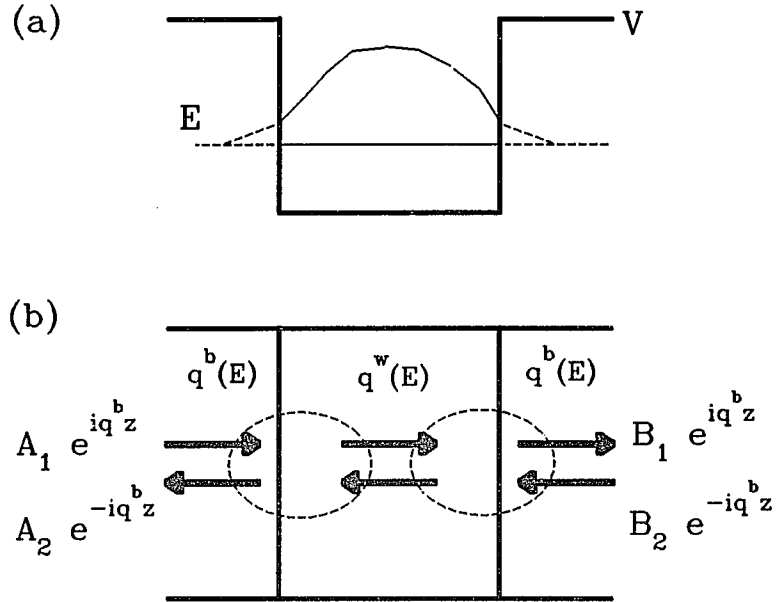


FIG. 13 Schematic diagram of a SQW structure in (a) potential and (b) q picture.

propagation through a multi-layer film. Thus a similar method to the optical matrix method can be developed. We will use the notation where all the variables associated with the well/barrier region are noted with the superscript w/b .

For SQW shown in Fig. 13, we define a system matrix $[S(E)]$ as:

$$\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = [S_{2 \times 2}(E)] \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \quad (4.43)$$

From the commutational property of the Hamiltonian and the time reversal operator, the $[S]$ matrix has the following property,

$$S_{11} = S_{44}^* \quad S_{12} = S_{21}^* \quad (4.44)$$

By defining the interface and propagating matrix similar to the optical matrix method, the system matrix $[S]$ can be evaluated.

$$\begin{aligned} [S_{2 \times 2}] &= \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = [M^b] \times [M^w]^{-1} \times [-L_z^w] \times [M^w] \times [M^b]^{-1} \\ &= \begin{bmatrix} 1 & 1 \\ Q^b & -Q^b \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ Q^w & -Q^w \end{bmatrix} \begin{bmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ Q^w & -Q^w \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ Q^b & -Q^b \end{bmatrix} \quad (4.45) \\ &= \frac{1}{4Q^wQ^b} \begin{bmatrix} (Q^w+Q^b)^2e^{-i\phi}-(Q^w-Q^b)^2e^{i\phi} & (Q^w-Q^b)(e^{-i\phi}-e^{i\phi}) \\ (Q^w-Q^b)(e^{i\phi}-e^{-i\phi}) & (Q^w+Q^b)^2e^{i\phi}-(Q^w-Q^b)^2e^{-i\phi} \end{bmatrix} \end{aligned}$$

where:

$$Q^w = \frac{q^w(E)}{m^w} \quad Q^b = \frac{q^b(E)}{m^b} \quad \phi = q^w(E)L \quad (4.46)$$

All the system characteristics including the energy levels can be found in this [S] matrix. Define the transmission probability $T(E) = \frac{1}{|S_{11}(E)|}$. For a SQW with well width

L_z and barrier height V_b , we have:

$$T = \frac{1}{\sqrt{1 + \left[\frac{1 - \gamma^2}{2\gamma} \sin \phi \right]^2}} \quad (E > V_b) \quad (4.47)$$

$$T = \frac{1}{\left| \cos \phi - \frac{1 - \beta^2}{2\beta} \sin \phi \right|} \quad (0 < E < V_b)$$

where:

$$\gamma = \sqrt{\frac{m^w}{m^b} \frac{E - V_b}{E}}$$

$$\beta = \sqrt{\frac{m^w}{m^b} \frac{V_b - E}{E}} \quad (4.48)$$

$$\phi(E) = \frac{L_z}{\hbar} \sqrt{2m^w E}$$

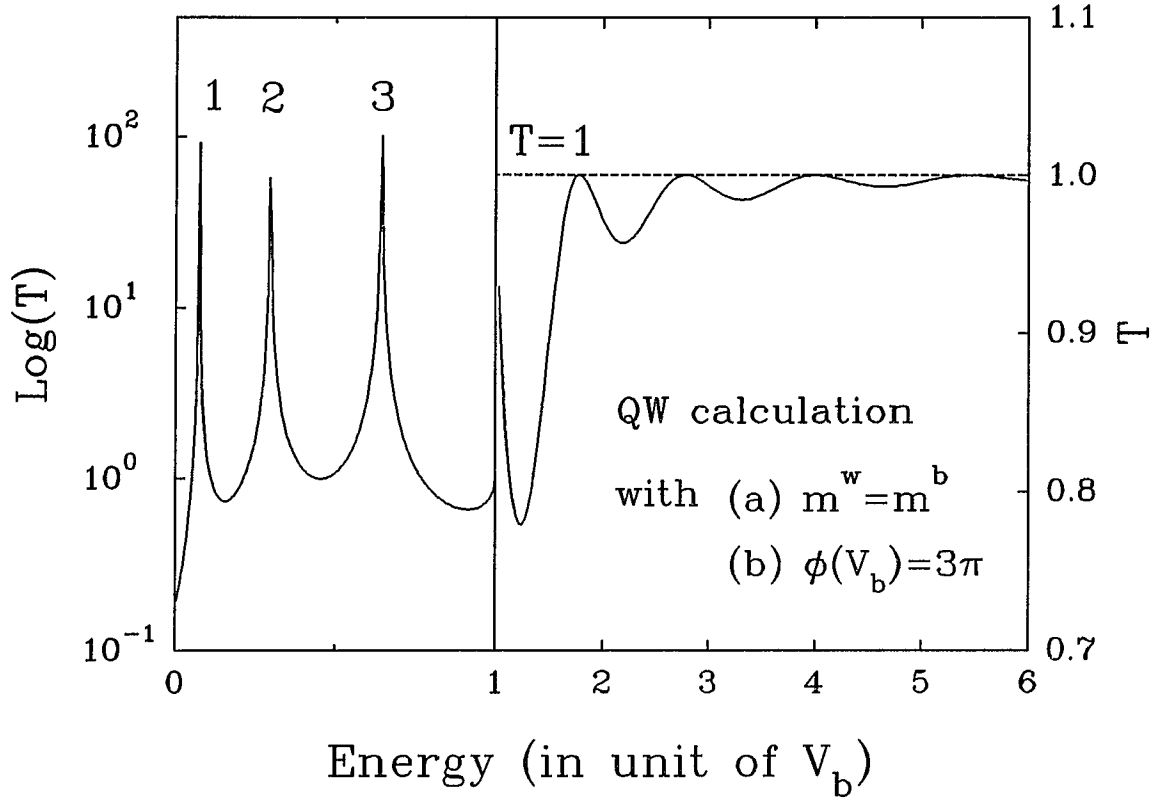


FIG. 14 Calculated $T(E)$ of QW structures with (a) $m^w = m^b$ and (b) $\phi(V_b) = 3\pi$.

The calculated $T(E)$ is shown in Fig. 14 for a SQW with $m^w = m^b = m$ and $\phi(V_b) = 3\pi$. Three discrete bound states are observed as $T \rightarrow \infty$ sharp lines (singularities) below barrier height ($0 < E < V_b$), which agrees with the results of modified Kronig-Penny model determined by $\tan\phi = 2\beta/(1-\beta^2)$. The resonance behavior is also observed above the barrier height ($E > V_b$) where 100% transmission efficiency is permitted.

Thus the matrix method offers an alternative way of obtaining the resonance energy positions, and this approach can be easily extended to the coupled two level systems.

4.4.2 Coupled Two-Level QW System

Shown in Fig. 15 is a schematic diagram of a coupled two-level SQW system. We need to solve two problems in this situation, the $q(E)$ dispersion and the calculation of the various matrices.

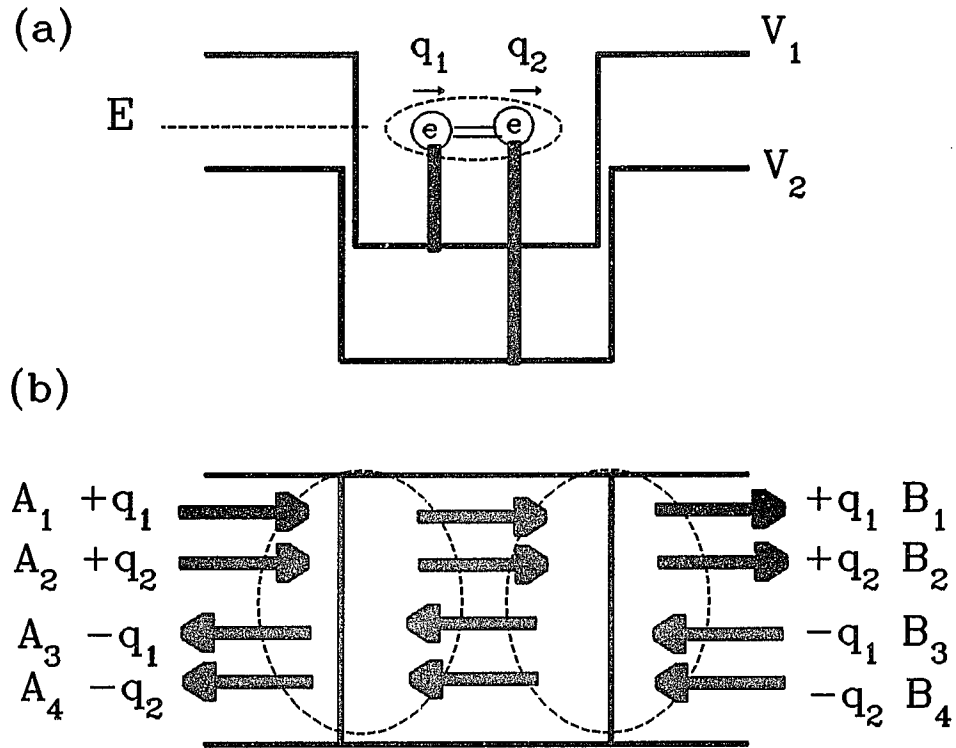


FIG. 15 Schematic diagram of a coupled two level SQW system.

There will be two normal modes $q_1(E)$ and $q_2(E)$ propagating in both levels. The proper description of the dynamical picture will need four plane waves, $\exp(\pm iq_1 z)$ and $\exp(\pm iq_2 z)$.

The calculation of the matrices involves only linear algebra. The $[S]$ matrix now becomes a 4×4 matrix,

$$\begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = [S_{4 \times 4}(E)] \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} \quad (4.49)$$

We can obtain the $[S]$ matrix in similar way as SQW in previous section. For simplicity, we will not discuss the mathematical details here. With the introduction of some new parameters which have more direct physical meanings, we can extract the information of the resonance energy levels from the $[S]$ matrix. One such quantity is the $[T]$ matrix defined as,

$$[T_{2 \times 2}] = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}^{-1} \quad (4.50)$$

The physical meaning of this matrix is illustrated in Fig. ?. A calculated example of zero coupling has been shown in Fig. 14, and a more detailed example of in-plane uniaxial stress effect will be discussed in next section.

4.4.3 A Calculation Example

The coupling between two valence bands can be caused either by an in-plane uniaxial stress or by a finite k_x (or k_y) in the in-plane dispersion curve calculation or

some other means. The resulted coupling system can be treated by the very same technique we developed here.

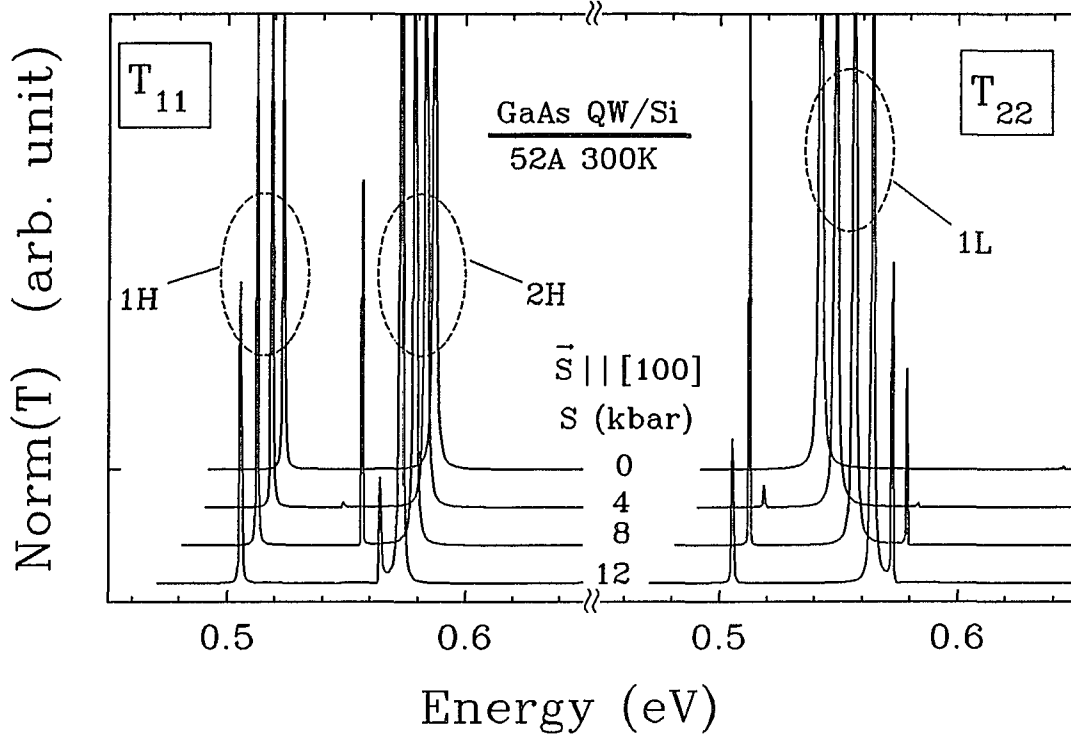


FIG. 16 Calculated T_{11} and T_{22} for the valence bands of a 52Å GaAs QW/Si structure under $S \parallel [100]$ for $S=0, 4, 8$, and 12 kbar.

As an example, the calculated $T_{11}(E)$ and $T_{22}(E)$ are shown in Fig. 16 for a 52Å GaAs SQW/Si structure under $S \parallel [100]$ for $S=0, 4, 8$, and 12 kbar (see section 7.3.4 for the experimental results). The different elastic constants of the GaAs (AlGaAs) layers and the Si substrate have been taken into account. This is a relatively clean system due to the narrow well width. At zero stress, the level 1 (HH) and level 2 (LH) are decoupled. The strong 1H and 2H resonances are observed only in the T_{11} curve, while the opposite is true for the 1L feature. As stress increases, the HH features

redshifted a little, which is due to an artifact that the conduction band has assigned certain portion of the contribution to the hydrostatic component. Net changes of the HH features relative to the conduction band are very small. On the other hand, from the T_{22} curves the 1L feature shows clearly a big blue shift under the stress. Besides the different stress dependence of the energy positions of the HH and LH features can be observed, the stress induced coupling can also be observed from the merging LH (HH) resonance in the T_{11} (T_{22}) curves as the stress increases. The coupling strength also reveals on the cross coupling elements such as T_{12} and T_{21} , which are not shown here. The cross-over between HH and LH features of the same parity can be observed on QW structures with wider well width, which we do not have in this example. The calculated transition energies for the 52Å GaAs SQW/Si sample in comparison with the experimental results can be found in Fig. 62 and Fig. 63, which shows an excellent agreement. More calculation results can be found in section 7.3.

Chapter 5. Temperature Effect

5.1 Introduction

The ability to perform modulation spectroscopy over a wide temperature range, particularly at elevated and room temperatures, has many fundamental as well as applied ramifications. Systematic studies of the effects of temperature on modulated spectra of various microstructures could reveal important information such as the dependence of transition energies and broadening parameters.

As the temperature of a semiconductor increases, the lattice expands and the phonon occupation number increases. The influence on the bulk energy gap due to lattice thermal expansion is similarly to what a hydrostatic pressure does. On the other hand, the increased phonon population will also shift the band edges through electron phonon perturbations. For most materials, either effect lowers the band gap. Temperature dependence of the fundamental absorption edge for many semiconductors has been described by a phenomenological classical equation proposed by Varshni (1967) involving three parameters:

$$E(T) = E(0) - \frac{\alpha T^2}{\beta + T} \quad (5.1)$$

where $E(0)$ is the energy gap at zero temperature, α and β are two adjustable parameters.

This equation reflects that the temperature dependence of energy gap is (a) linear ($\propto \alpha T$) at high temperatures and (b) quadratic, $\propto (\alpha/\beta)T^2$, at low temperatures. The

transition region is characterized by temperature β . Recently another relation has been proposed by Lautenschlager *et al* (1987a, 1987b), which contains the Bose-Einstein occupation factor for the phonons:

$$E(T)=E(0)-\frac{2a_B}{e^{\frac{E_{ap}}{k_B T}}-1} \quad (5.2)$$

where $E(0)$ is the energy gap at zero temperature, E_{ap} is the effective phonon energy usually dominated by acoustical phonon contributions, and a_B is the electron phonon coupling parameter.

Besides this shift of band edges, energy levels are broadened proportionally to the phonon population (P. Lautenschlager *et al*, 1987a):

$$\Gamma(T)=\Gamma_0+\Gamma_{ep}N_{ph}(T) \quad (5.3)$$

where $\Gamma_0=\Gamma(T=0)$ and Γ_{ep} (electron-phonon coupling coefficient) are two fitting parameters, and $N_{ph}(T)$ is the phonon occupation number at temperature T . The other temperature dependent contributions such as the impurity scattering and the acoustic phonon scattering are omitted since they are relatively small. Since phonons are Bosons, they obey the Bose-Einstein statistics:

$$N_{ep}(T)=\frac{1}{e^{\frac{E_{ph}}{k_B T}}-1} \quad (5.4)$$

here, the E_{ph} is the relevant phonon energy. It has been shown from both the theoretical and experimental works that the relevant phonon is the longitudinal optical (LO) phonon near Brillouin zone center.

In section 5.3.1, we show as an example the temperature dependence of fundamental band gap $E_0(T)$ and its associated broadening parameter $\Gamma(T)$ of a bulk GaAs sample.

In going from three dimensional bulk case to reduced dimensional systems such as pseudo two dimensional SQW structures, these relations have shown to be still valid. In section 5.3.2, we will confirm this on a high quality InGaAs/GaAs SQW structure. Attention will also be paid to the appropriate MS line shape functions at different temperatures.

In semiconductor microstructures such as SQWs, besides the similarity to bulk materials on the qualitative temperature dependence, new phenomena may occur as both electrons and phonons are now confined. Our work on several InGaAs/GaAs and GaAs/AlGaAs QWs shows that although the quantitative temperature dependence of QW transition energies generally follow the band edge of the constituent bulk material of well region, $\Gamma(T)$ becomes less sensitive to temperature as the dimensionality of the system is reduced. We show that temperature variation of the broadening parameter $\Gamma(T)$ of exciton features of quantum structures offers an interesting way to explore the

dependence of electron-phonon interaction on dimensionality. We found an approximately linear reduction of the coupling coefficient Γ_{cp} on dimensionality in the range $50\text{\AA} < L_z < 200\text{\AA}$. The findings of reduced electron (exciton)-phonon coupling in reduced dimensional system will be discussed in section 5.3.3 on a series of GaAs/AlGaAs SQW structures. Possible tuning of this coupling in a reduced dimensional system will also be demonstrated in section 5.3.4 by an example of insertion of several AlAs monolayers at the QW interfaces.

5.2 Experimental Setup

The temperature variation below 300K is achieved on a open cycle cryogenic system with optical access of Model LT-3-110 Heli-Tran[®] Liquid Transfer Refrigeration System made by Air Products and Chemicals, Inc., which is capable of operation below 4.2 K. Temperature variation is stabilized within 0.1 K by a matching Series 3700 Digital Temperature Indicators/Controllers from the same company.

High temperature experiments are performed on a home made system. The variation of temperature is achieved by adjusting heating power, which is capable of going above 600 C. The heat dissipation channel is relatively stable in the closed laboratory environment, so no feed back temperature control loop is used. Typical temperature variation on the thermal couple reading during a spectrum collection is within one degree.

5.3 Experimental Results

5.3.1 Temperature Effects on Bulk GaAs

As an example, PR spectra around fundamental absorption edge E_0 of a bulk GaAs sample at 6.6K, 80K, 210K, 295K, 380K, and 500K are shown in Fig. 17 as solid lines. The semi-insulating GaAs sample is a (001) commercial wafer fabricated by the liquid encapsulated Czochralski method. Such material is frequently employed as a substrate for

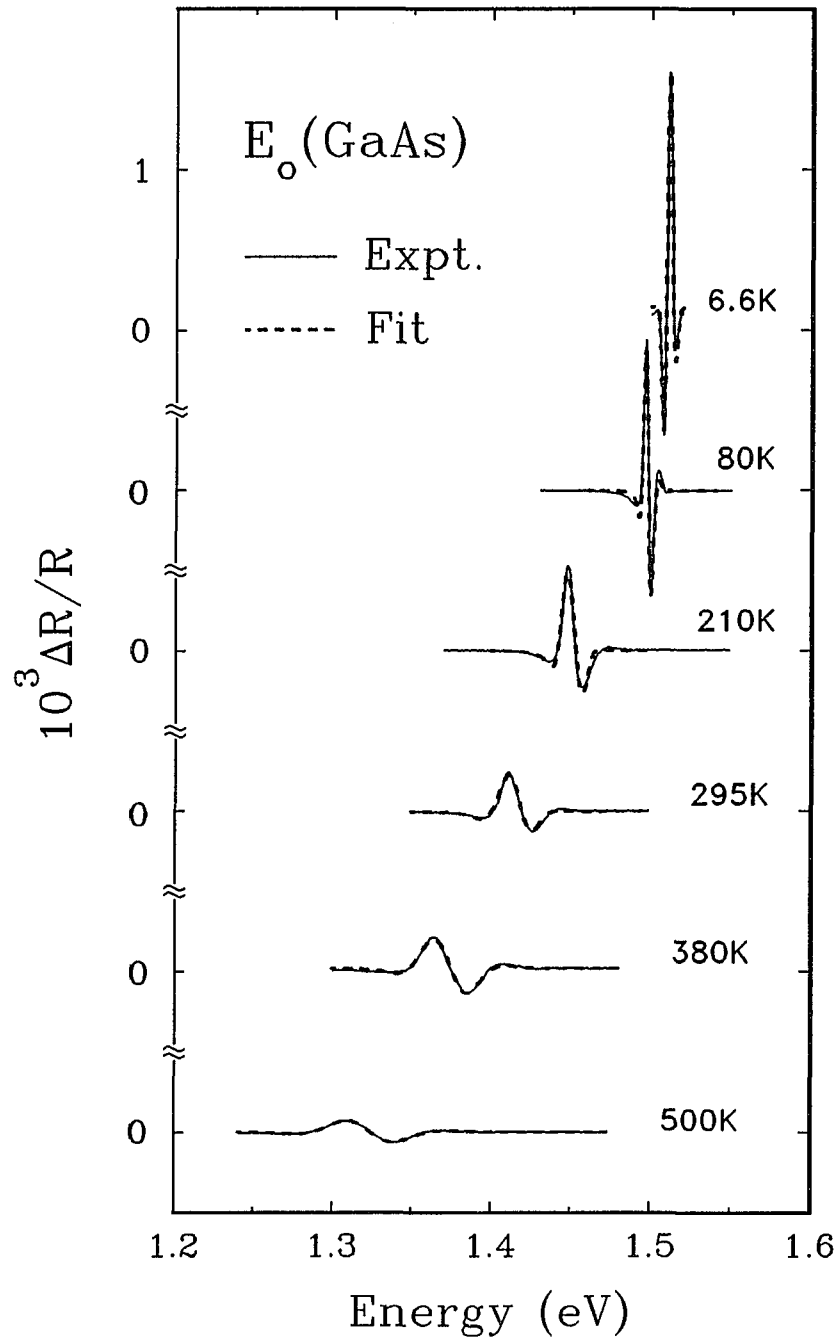


FIG. 17 PR spectra of a bulk GaAs at different temperatures.

the fabrication of various GaAs based thin film structures. No special treatment was given to the surface. Several changes can be seen on the experimental curves when temperature increases (a) E_0 peak position undergoes a monotonic red shift, (b) its associated linewidth increases and (c) signal amplitude reduces. The PR spectra were fit to the FDGL function, which are shown as dashed lines. The line shape fits yield accurate values of E_0 and Γ at different temperatures.

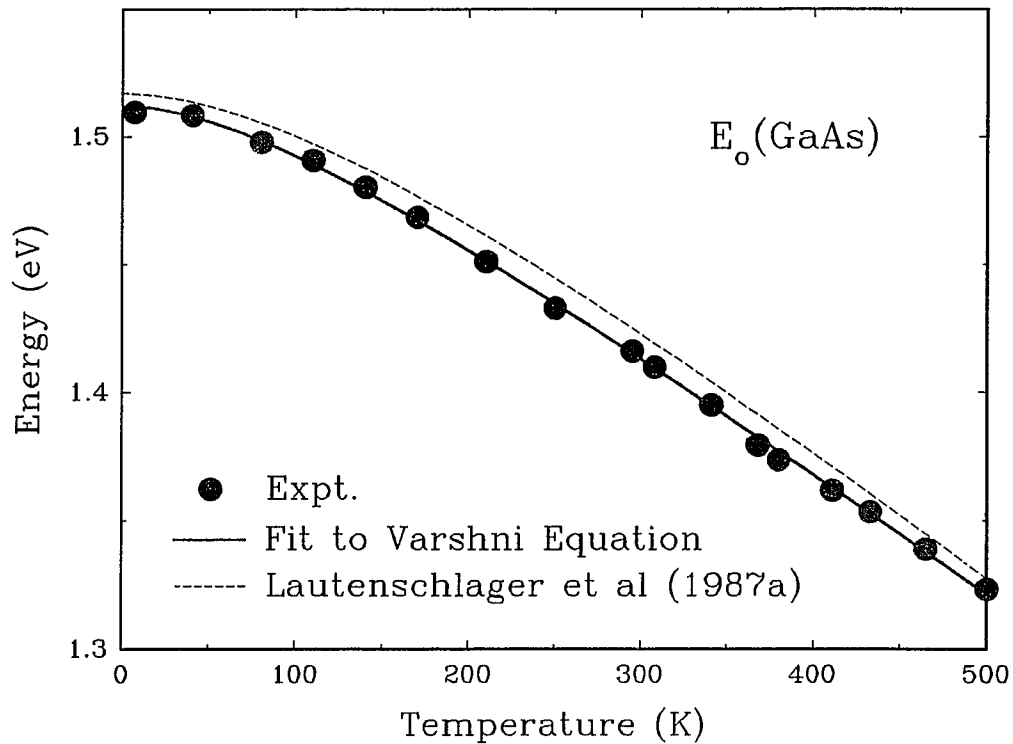


FIG. 18 Temperature dependence of the fundamental absorption edge E_0 of bulk GaAs.

The transition energies $E_0(T)$ at various temperatures obtained from least squares fits are shown in Fig. 18 as solid circles. The solid line is a least squares fit to Varshni's relation, Eq. (5.1). The satisfactory fit demonstrates the validity of this model on bulk

Table II Values of $E(0)$, α , β , and Γ_{ep} of the bulk GaAs.

	This Work	Previous Works
$E(0)$ (eV)	1.512 ± 0.003	1.517 ± 0.018^a 1.512^b
α (10^{-4} eV/K)	4.97 ± 1	5.5 ± 1.3^a 5.1^b
β (K)	150 ± 100	225 ± 174^a 190^b
Γ_{ep} (meV)	20 ± 1	48 ± 26^a 7^c 21^d

- a. P. Lautenschlager *et al* (1987a).
b. H. Shen *et al* (1988).
c. V. L. Alperovich *et al* (1976).
d. Calculation of S. Rudin *et al* (1990).

materials. Various parameters obtained from the fit are listed in Table II. Some previous experimental and theoretical results are also listed for comparison purposes. It should be noted that although the value of $E(0)$ can be determined accurately, the numbers of α and β have large error bars unless high temperature experiments are performed. For example, shown in the Fig. 18 as the dashed line is the result of Lautenschlager *et al* (1987a). It agrees with our experimental result (solid line) very well except for the $E(0)$ shift which is probably due to the exciton binding energy as well as the systematic error. But as shown in the Table II the difference of α (10%) and β (50%) is not so small.

Shown in Fig. 19 as solid circles are the broadening parameters, $\Gamma(T)$, obtained from the line shape fits. The solid line is the least squares fit to Eq. (5.3). This model

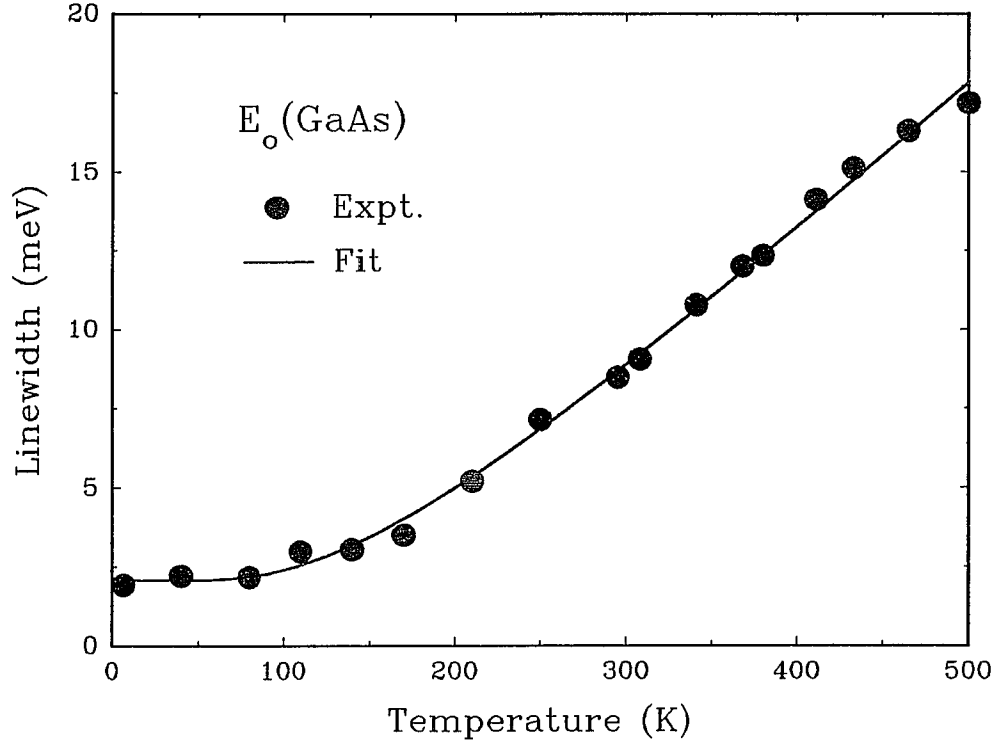


FIG. 19 Temperature dependence of the broadening parameter of the E_0 transition of bulk GaAs.

fits well to the experimental data. The parameter Γ_{ep} obtained from the fit are also listed in Table II together with some previous experimental and theoretical results. The Γ_{ep} of bulk GaAs has not been well established before. V.L. Alperovich *et al* (1976) reported 7meV from the absorption measurement. However, this result has large error bars which is evident from the small $\Gamma(295K)=4meV$ extracted from the very broader absorption edge. Our value agrees well with the spectroscopy ellipsometry result (P. Lautenschlager *et al*, 1987a). The smaller error bar of our result is due to the assumption that the relevant phonon energy is exactly the LO phonon energy, which has been confirmed by many experimental and theoretical works. Our value also agrees very well with the calculation of S. Rudin *et al* (1990).

The question of whether these models are still valid for the fundamental transitions originating from semiconductor microstructures such as SQWs will be examined in the following section.

5.3.2 Temperature Effects on Semiconductor Microstructures and Modulation

Spectroscopy Line Shape Changes (InGaAs/GaAs Strained SQW)

During the past several years there has been considerable interest in the strained layer InGaAs/GaAs system from both fundamental and applied points of view. Strained layer heterostructures utilize constituent layers with unequal lattice constants. When the thickness of the layers is below a critical value, the lattice mismatch can be accommodated by elastic strain and thus the growth of dislocation-free structures can be achieved (see for example J. W. Mayer and S. S. Lau, 1990). This freedom from the need for precise lattice matching widens the choice of compatible materials and greatly increases the ability to control the optical and electronic properties of such structures. For thin layers grown pseudomorphically, the strain induces a significant change in the electronic band structure. This makes it possible to control the band gap and the associated quantum transitions by altering the ternary composition (strain) and layer thickness (confinement). Advantages of such a strained layer system include not only band gap tailoring for long wavelength lasers (W. T. Tsang, 1987) but also the exploitation of the light in-plane hole mass and high electron peak velocities for horizontal structures such as high electron mobility transistors (H. Morkoc and H. Unlu, 1987).

We have carried out a study of the temperature dependence of the PR spectra from a strained layer (001) $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW in the range $10\text{K} < T < 500\text{K}$ (Y. S. Huang *et al*, 1991b; H. Qiang *et al*, 1992a). Special attention has been paid to the fundamental 11H exciton transition. From a detailed line shape fit we have obtained the variation with temperature of the 11H energy gap $E_{11\text{H}}(T)$ as well as its broadening parameter $\Gamma(T)$. The InGaAs/GaAs system is ideally suited for such an investigation since the strain increases the separation between the heavy and light holes in relation to the comparable GaAs/AlGaAs quantum wells. Thus, in contrast to the latter heterostructure, there is no overlap between the 11H and 11L PR features in this system for the well width (L_z) used in this study (100Å).

The InGaAs/GaAs SQW was fabricated by molecular beam epitaxy in a Varian Gen-II system at IBM T. J. Watson Research Center. The growth conditions indicated an In composition of 20% and a well width of 100Å.

Shown by the solid lines in Figs. 20(a) and 20(b) are the experimental PR data in the region of the 11H transition at 10K. The dotted line in Fig. 20(a) is a least squares fit to FDLL function [Eq. (3.8) and Eq. (3.14)] using a single oscillator. The fit appears to be quite good yielding the value of the exciton energy $E_{11\text{H}}$, indicated by the arrow at the bottom of the figure, and the broadening parameter Γ . The dashed line in Fig. 20(b) is a least squares fit to a FDGL function [Eq. (3.12) and Eq. (3.13)] considering only the energy gap modulation mechanism. Again the agreement with

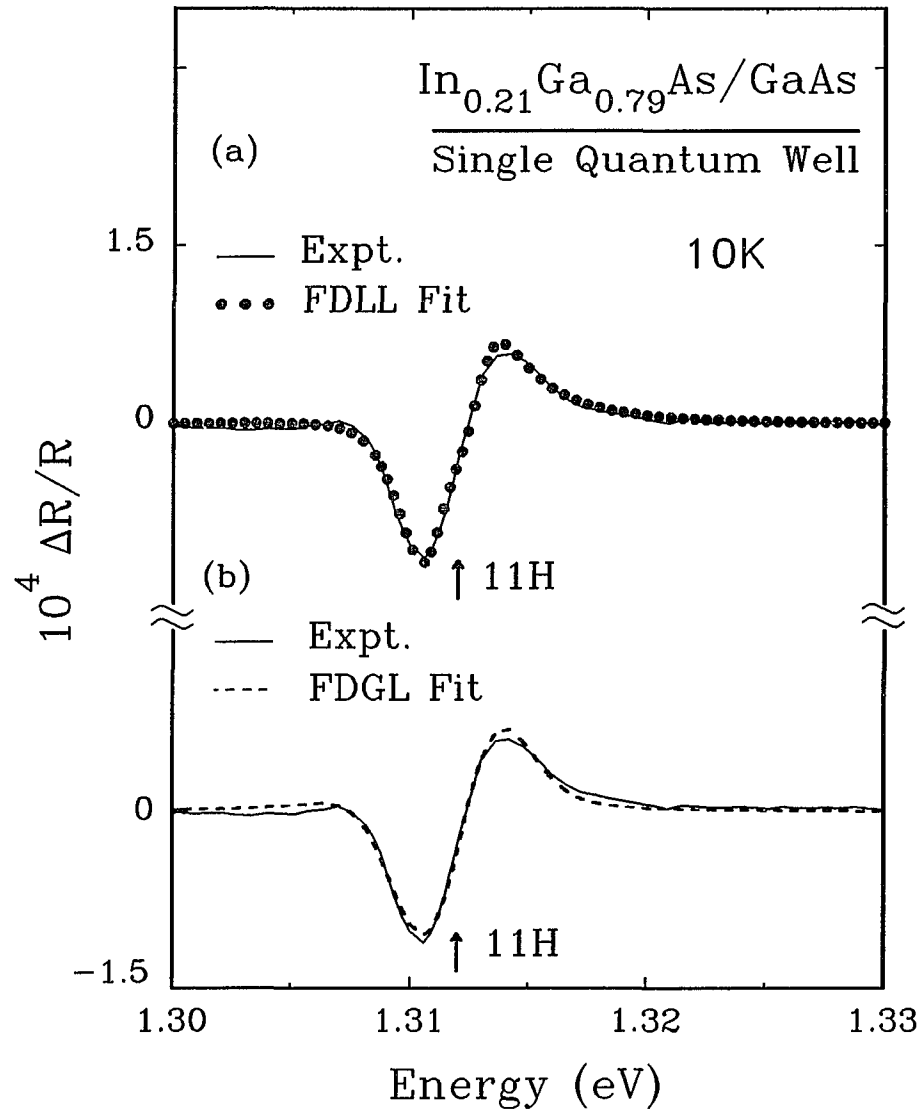


FIG. 20 Experimental PR spectrum (solid line) in the region of the 11H transition of an InGaAs/GaAs SQW ($L_z=105\text{\AA}$) at 10K. The dotted and dashed lines are FDLL and FDGL fits, respectively.

experiment is quite good yielding Γ and the energy position indicated by the arrow. Note that the two line shapes yield almost the same energy position E_{11H} and Γ values. We also attempted a fit to the line shape function of a 2D CP (Eq. (3.15) with $n=3$) but it gave a much worse result than either of the above excitonic line shapes.

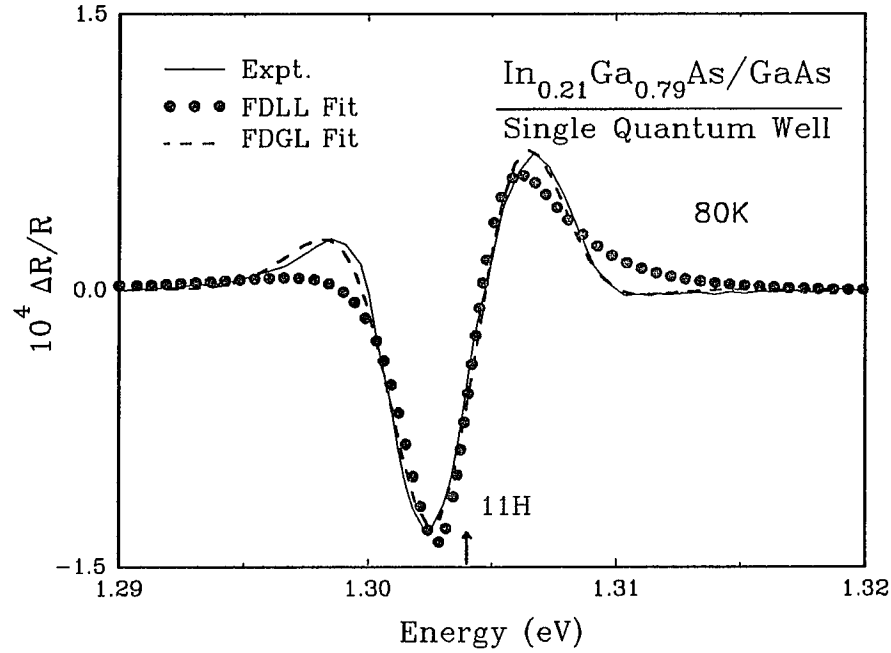


FIG. 21 Experimental PR spectrum (solid line) in the region of the 11H transition of an InGaAs/GaAs SQW ($L_z=105\text{\AA}$) at 80K. The dotted and dashed lines are FDLL and FDGL fits, respectively.

Displayed in Fig. 21 by the solid line is the 11H PR spectrum at 80K. Note the low energy wing in relation to the data of Fig. 20. The dotted and dashed lines are least squares fits to FDLL and FDGL, respectively, using a single oscillator. For the latter case both energy gap and broadening modulation mechanisms were needed. Clearly the FDGL yields a much better fit, particularly in the low energy wing.

In Fig. 22 is plotted the experimental PR data (solid line) in the region of 11H at 300K. Note that the spectrum is asymmetric on the high energy side, in contrast to the symmetric line shapes of Figs. 20 and 21. The dotted line is a least squares fit to a FDGL function using only one oscillator. The fit on the high energy side of the feature is not very good indicating the presence of a second oscillator. Shown by the dashed line

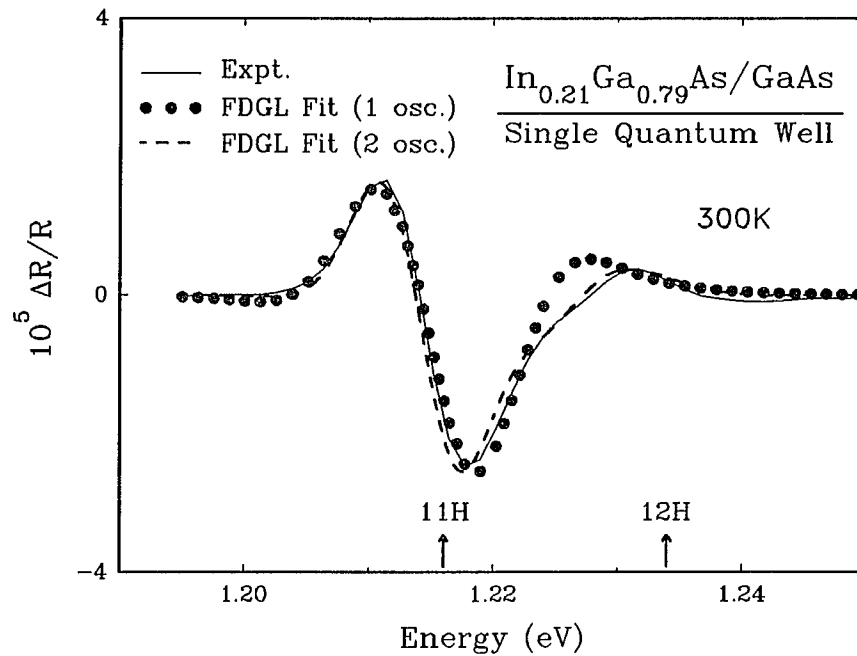


FIG. 22 Experimental PR spectrum (solid line) in the region of the 11H transition of an InGaAs/GaAs SQW ($L_z=105\text{\AA}$) at 300K. The dotted and dashed lines are FDGL fits (see text).

is a FDGL fit using two oscillators. At this temperature 11H has become sufficiently broad so that it overlaps the second oscillator, 12H transition. The obtained energies are designated by arrows. The justification for attributing the second oscillator to the "symmetry forbidden" 12H transition is confirmed by the low temperature data where 12H is clearly resolved.

The FDGL (possible FDLL at low temperature) function provided a good fit to the PR data, up to 500K, indicating the excitonic nature of 11H up to this temperature.

The first-derivative nature of the line shapes in Figs. 20-22 are consistent with the considerations of Glembocki and co-workers (O.J. Glembocki *et al*, 1987; B.V.

Shanabrook *et al*, 1987). For a low dimensional system the spectra should be the first derivative of an excitonic profile which is Gaussian at temperatures where the electron-phonon interactions becomes important. For $T > 80\text{K}$ the PR spectra of 11H are the first derivative of a Gaussian profile while at low temperature (10K) the data can be fit to either FDGL or FDLL (see Fig. 20). This result is somewhat different than that reported for 11H of a GaAs/AlGaAs MQW (O.J. Glembocki *et al*, 1987), where the spectrum was FDLL at low temperatures (6K) and then evolved to FDGL as the temperature was increased. Our spectrum of Fig. 20 is probably FDGL since (a) the constituent material in the well is an alloy, (b) Γ_0 is approximately equal to the value deduced from a theory based on statistical alloy fluctuations (J. Singh and K.K. Bajaj, 1986) and (c) there is no significant broadening change between 10K and 80K [$\Gamma(10\text{K}) \approx \Gamma(80\text{K})$] and it is FDGL at 80K (see Fig. 21). These results indicate that care must be taken in associating the absence of pronounced wings in the spectra with a FDLL (O.J. Glembocki *et al*, 1987). The fact that our 11H line shape is FDGL demonstrates the excitonic nature of this transition even up to 500K.

The temperature dependence of $E_{11\text{H}}$ is plotted in Fig. 23. The solid line is a least squares fit to the semiempirical Varshni expression [see Eq. (5.1)]. The satisfactory fit demonstrates the validity of this model in semiconductor microstructures. Listed in Table III are the obtained values of $E(0)$, α and β . For comparison purposes we also display recently measured values of the direct gap for strain relieved $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ ($x=0.06$ and 0.15) bulk material by Z. Hang *et al* (1991).

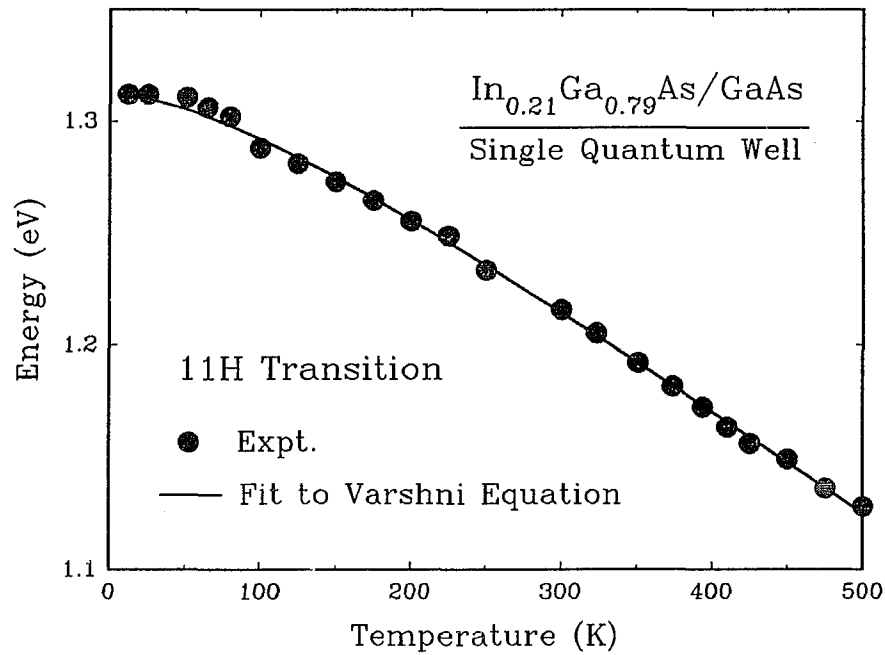


FIG. 23 Temperature dependence of the 11H transition of an InGaAs/GaAs SQW ($L_z=105\text{\AA}$). The solid line is a least squares fit to Varshni equation [Eq. (5.1)].

From Table III it can be seen that α and β for 11H in our sample are fairly similar to bulk $\text{In}_x\text{Ga}_{1-x}\text{As}$ ($x=0.06$ and 0.15). Therefore, as in the GaAs/AlGaAs heterostructure system the main influence of temperature on the quantized transitions is

Table III Values of $E(0)$, α and β of the 11H transition in an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW.

Material	$E(0)$ (meV)	α (10^{-4} eV/K)	β (K)
$\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW ^a	1312 ± 5	4.8 ± 0.3	140 ± 40
$\text{In}_{0.06}\text{Ga}_{0.94}\text{As}$ bulk ^b	1420 ± 5	4.8 ± 0.4	200 ± 50
$\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$ bulk ^b	1285 ± 5	5.0 ± 0.4	231 ± 40

a. This work.

b. Z. Hang *et al* (1991).

through the temperature dependence of the band gap of the constituent material in the well (A. Kangarula *et al*, 1988).

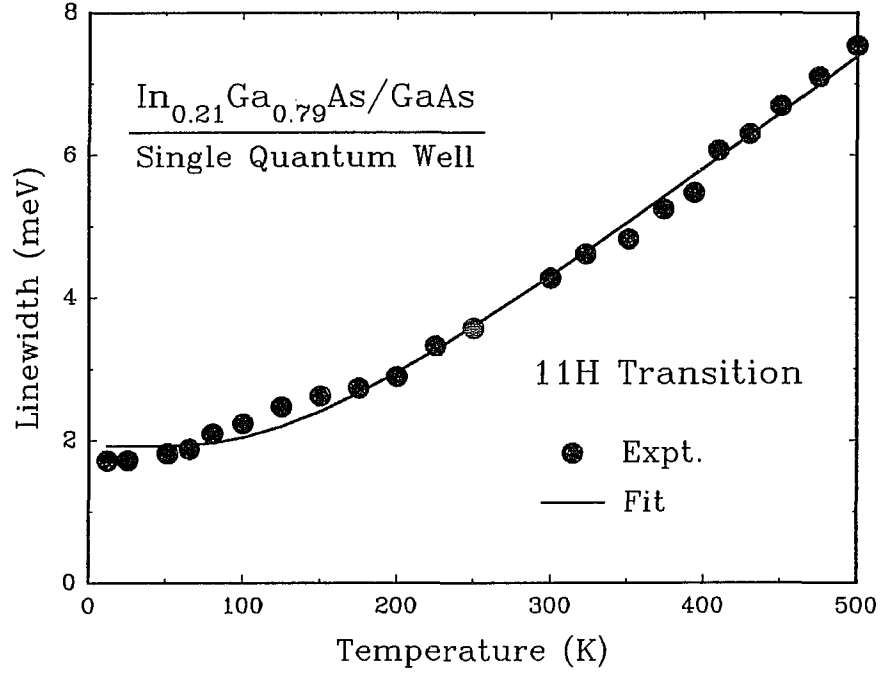


FIG. 24 Temperature dependence of the broadening parameter of the 11H transition of an InGaAs/GaAs SQW ($L_z=105\text{\AA}$). The solid line is a least squares fit to Eq. (5.3).

In Fig. 24 we display the temperature dependence of the phenomenological broadening parameter Γ as determined from the FDGL fit. The solid line is a least squares fit to the phonon coupling model given by equation (5.3). The satisfactory fit shows this model is still valid in semiconductor microstructures such as SQW. From the fit we obtained the value of $\Gamma_0=1.9\pm0.1\text{meV}$, $\Gamma_{\text{cp}}=6.9\pm0.5\text{meV}$.

Our measured number for Γ_0 is considerable smaller than those reported in literature (K. F. Huang *et al*, 1989) for somewhat similar SQWs. Our value of about

1.9meV is close to the theoretical limit for alloy scattering (J. Singh *et al*, 1986), which may be the reason of FDGL down to low temperature. This fact indicates the structural high quality of the material (uniform strain distribution) and interface, averaged over the region sampled by the exciton Bohr radius ($\sim 50\text{\AA}$).

The obtained value Γ_{ep} is somewhat smaller than those reported on the bulk InGaAs (Z. Hang *et al*, 1991). A systematic study on this phenomenon was carried out on a series of GaAs/AlGaAs SQW structures. These results will be discussed in the following section.

The results also show that FDGL in addition to FDLL (at low temperatures in certain cases) are the appropriate line shape functions to describe the exciton features of semiconductor microstructures.

5.3.3 Exciton-Confined LO Phonon Interactions in Reduced Dimensional Systems (GaAs/AlGaAs SQW)

The coupling between photons and elementary excitations such as electrons and excitons is an important parameter in determining many of the electronic and optical properties of semiconductor microstructure. There has recently been considerable interest in the electron (exciton) -optical phonon coupling in reduced dimensional polar semiconductor systems such as heterojunctions, quantum wells, quantum wires, quantum boxes, and nanospheres. In these systems the electron (exciton)-optical phonon

(Frohlich) interaction is affected not only by changes in the particle wave function due to the confining potential but also by changes in the longitudinal optical (LO) phonon modes caused by phonon confinement. The changes from bulk material are evidenced by the results of Γ_{ep} in preceeding section. Although there have been a number of theoretical treatments (S. Rudin and T. L. Reinecke, 1990a, 1990b, 1991), there have been relatively few experimental results. The time-dependent Raman scattering results of Kim and Yu (1990) and Tsen *et al* (1991) on GaAs/AlGaAs MQWs of different well widths were explained in terms of confinement of both the electrons and optical phonons in the quantum wells. Interband relaxation in GaAs/AlGaAs MQWs has been detected by an infrared bleaching technique (A. Seilmeier *et al*, 1987). The size dependence of the exciton-LO phonon coupling in CdSe (M. C. Klein, 1990) and CuCl (Y. Masumoto *et al*, 1989) nanospheres has been reported.

Electron (exciton) -LO phonon coupling strength can be evaluated by studying the phonon population dependence of the linewidth $\Gamma(T)$ of the fundamental absorption edge in reduced dimensional system. One way to tune the phonon population precisely and conveniently is by varying the sample lattice temperature. In both bulk and low-dimensional systems the dominant mechanism for the temperature dependence of linewidth (thermal broadening) is the interaction with the LO phonons. Thus, $\Gamma(T)$ can be described by a Bose-Einstein relation which contains a coupling constant Γ_{ep} [see Eq. (5.3)]. Several workers have measured $\Gamma(T)$ for the fundamental conduction to heavy-hole intersubband excitonic transition (11H) in GaAs/AlGaAs MQWs (Y. Chen *et al*,

1987; S. Selci *et al*, 1991; D. Miller *et al*, 1982; O. J. Glembocki *et al*, 1986) and an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW (Y. S. Huang *et al*, 1991), and have extracted values of Γ_{ep} . However, these authors did not present firm conclusions concerning the dimensionality dependence of Γ_{ep} . This is probably because these studies were (a) not systematic and (b) Γ_{ep} for the bulk constituent material of the well was not well established.

We have carried out a systematic PR study (H. Qiang *et al*, 1992c) of the temperature dependence ($10\text{K} < T < 500\text{K}$) of $\Gamma(T)$ of the fundamental absorption edge of bulk GaAs (E_0) and 11H of five MBE grown $\text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ SQWs with different well width ($60\text{\AA} < L_z < 200\text{\AA}$). We have observed a monotonic decrease of Γ_{ep} with reduced dimensionality and size. The value of Γ_{ep} for E_0 of bulk GaAs is considerably larger than Γ_{ep} of our five $\text{GaAs}/\text{AlGaAs}$ SQWs and the $\text{GaAs}/\text{AlGaAs}$ MQWs reported in the literature (Y. Chen *et al*, 1987; S. Selci *et al*, 1991; D. Miller *et al*, 1982; O. J. Glembocki *et al*, 1986). In our five $\text{GaAs}/\text{AlGaAs}$ SQW samples, it is found that Γ_{ep} scales linearly with L_z . We interpret our observations as evidence for the size dependence of the electron (exciton) -LO phonon interaction in reduced dimensional systems.

The SQW samples were grown by MBE on GEN-II at University of Glasgow. The first series consists of five samples grown at identical conditions with varying $L_z = 60, 80, 120, 130, 200\text{\AA}$. A three mono-layer AlAs layer was placed at either $\text{GaAs}/\text{AlGaAs}$ interface.

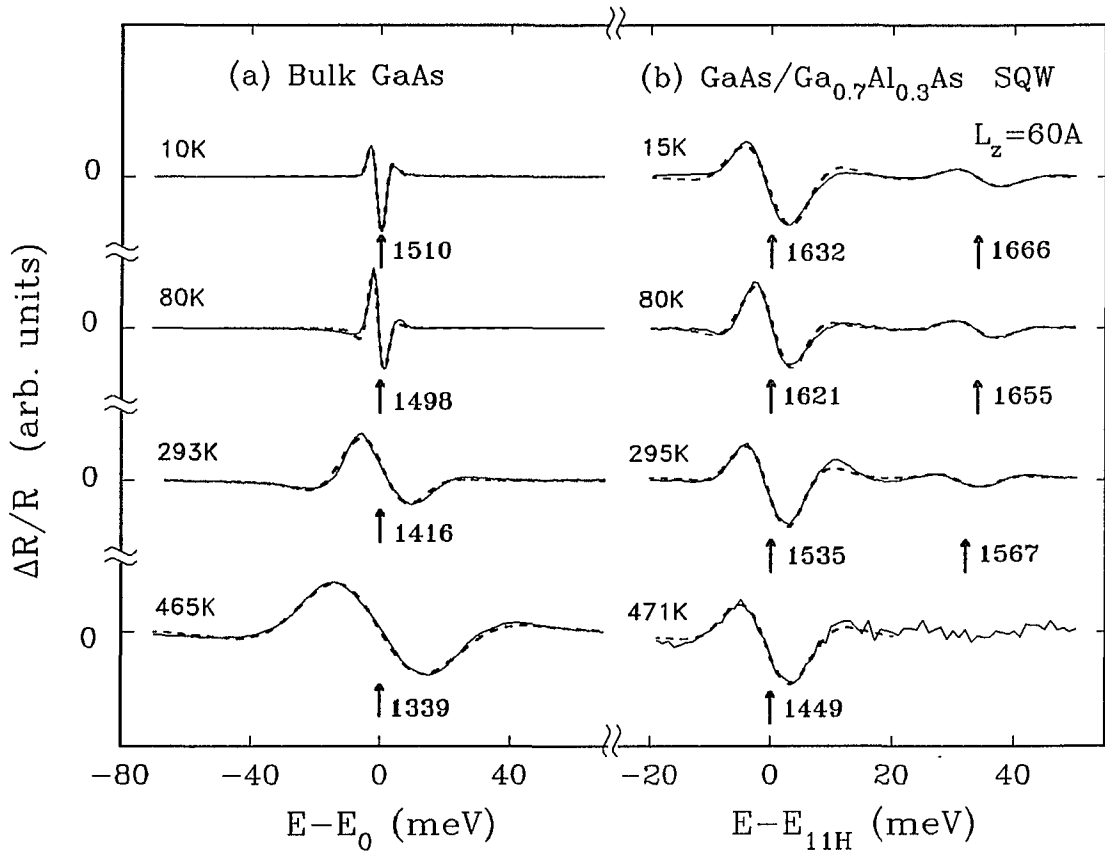


FIG. 25 Experimental PR spectra at various temperatures around (a) E_0 of bulk GaAs and (b) 11H and 11L of a GaAs/Al_{0.3}Ga_{0.7}As SQW ($L_z=60\text{\AA}$).

Shown by the solid lines in Fig. 25(a) are the PR traces of bulk GaAs in the region of E_0 for $T=10, 80, 293$, and 465K . To facilitate comparison of the spectra at different temperatures, we have taken the zero of energy of each scan to lie at the energy of E_0 . The dashed lines are least squares fits to a FDGL function. This fit has enabled us to accurately determine E_0 , as indicated by the arrows, as well as the quantity of interest, $\Gamma(T)$. The numbers next to the arrows are E_0 in meV. The first derivative nature of the line shape is indicative of an exciton. Band to band transitions would produce a third derivative spectrum.

The PR signal from the SQW with $L_z=60\text{\AA}$ in the region of 11H at $T=10, 80, 295$, and 471 K are indicated by the solid lines in Fig. 25(b). Again, we have taken the zero of energy to be the energy of the fundamental gap, i.e., E_{11H} . The higher lying feature is the fundamental electron-light hole exciton transition, 11L. The linewidths of these quantum transition features change only slightly with temperature. The dashed lines are least squares fits to a FDGL function (Eq. (3.12)). The obtained energies of 11H and 11L are indicated by the arrows and numbers in meV. The line shape fit also yields $\Gamma(T)$ for these two transitions.

Other workers have reported a change from Lorentzian to Gaussian first derivative for the 11H line shape in GaAs/AlGaAs MQWs as the temperature is increased (O. J. Glembocki, 1990; A. J. Shields *et al*, 1989). However, our 11H spectra are FDGL even at low temperatures, similar to the corresponding feature in the alloy InGaAs/GaAs SQW system as discussed in the previous section. This is probably a result of inhomogeneous broadening, which in our case may be due to effects such as microscopic well width fluctuations (interface roughness).

The temperature dependence of $\Gamma(T)$ for E_0 of bulk GaAs in addition to the 11H transition of two of the SQWs ($L_z = 200$ and $60\text{ \AA}$) are displayed in Fig. 26. For clarity we have displaced the curves and omitted the results for the $L_z = 130, 120$, and $80\text{ \AA}$ materials which fall between the curves of $L_z=200$ and $60\text{ \AA}$. The solid lines are least squares fits of Eq. (5.3) to the data (solid circles) for bulk GaAs and the two SQWs with

$E_{LO}=36\text{meV}$. We have neglected the small dependence of E_{LO} ($<0.5\text{meV}$) on temperature (J. Menendez and M. Cardona, 1984) and L_z (A. K. Arora *et al*, 1987).

The experimental values of Γ_{ep} of various L_z are displayed in

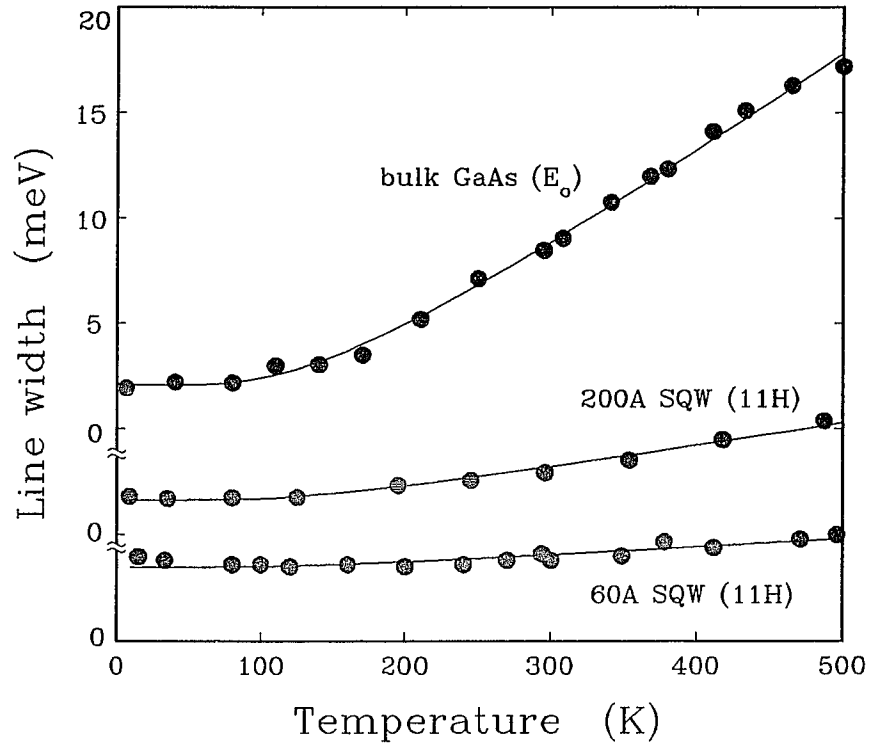


FIG. 26 Temperature dependence of $\Gamma(T)$ for E_0 of bulk GaAs and 11H transition of two SQWs with $L_z=200$ and $60 \text{ \AA}$.

Table IV. For bulk GaAs we find $\Gamma_{ep}=(20\pm1)\text{meV}$, in good agreement with the calculation of S. Rudin *et al* (1990). It is clear that the thermal broadening, i.e., electron (exciton) -LO phonon interaction, has been significantly suppressed as we move from bulk GaAs to reduced dimensional systems.

We have plotted Γ_{ep} as a function of L_z for our five SQW samples in Fig. 27. Note that there is a monotonic decrease of the Γ_{ep} as the dimensionality (L_z) is reduced, which is mainly a linear dependence. The dashed line is a least squares fit to a linear function drawn through the origin.

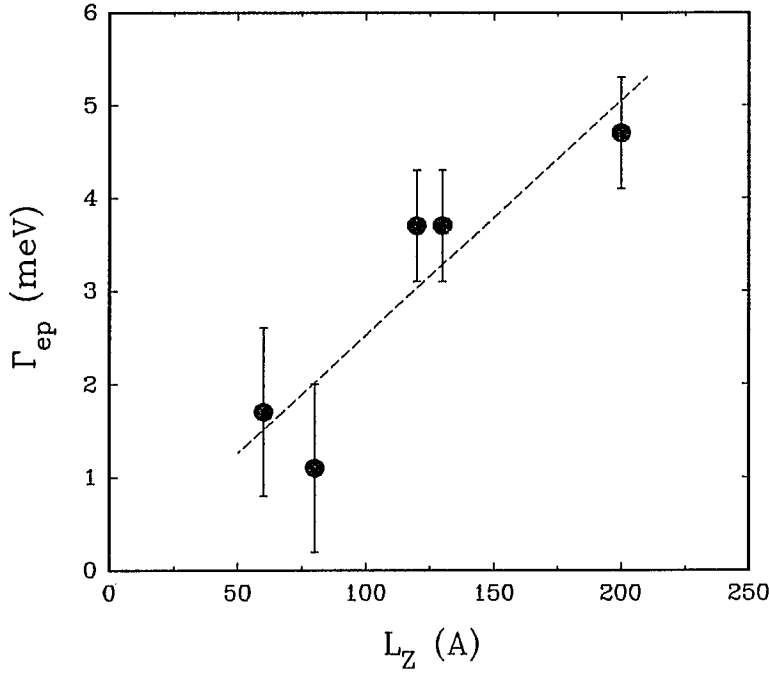


FIG. 27 Experimental electron (exciton) -LO phonon coupling constant Γ_{ep} as a function of L_z for GaAs/AlGaAs SQWs with 3ML AlAs interface layers.

This linear dependence can be qualitatively understood from a scaling argument of Frohlich interaction in polar materials.

In III-V polar materials, Frohlich interaction, in particular with LO phonon, is more important than deformation

potential interaction. Thus the electron (exciton)-LO phonon coupling constant Γ_{ep}^i of i th feature can be written down from the Frohlich Hamiltonian H_{ep} as:

$$\Gamma_{ep}^i = \sum_f \Gamma_f^i \propto \sum_f | \langle f | H_{ep} | i \rangle |^2 \quad (5.5)$$

where Γ_f^i is the contribution from the scattering state $|f\rangle$, which can be expressed more explicitly as:

$$\Gamma_f^i = \left[\frac{4\pi e^2 E_{LO}}{V} \right] \left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right] \sum_q \frac{1}{q^2} M_{fi} \quad (5.6)$$

where E_{LO} , V , ϵ_∞ , ϵ_0 , and q are the LO phonon energy, effective volume for phonon propagation, absolute permittivity at high and low frequency limit, and phonon wave vector, respectively. The matrix element M_{fi} is defined by,

$$M_{fi} = | \langle f | (a_q + a_{-q}^+) \varphi_{ph}(q, r) | i \rangle |^2 \quad (5.7)$$

where the matrix element M_{fi} involves the electron (exciton) wavefunctions $|i\rangle$ and $|f\rangle$ and phonon wavefunction $\varphi_{ph}(q, r)$. The wavefunctions are related to an allowed process which is governed by the operators a (anti-Stokes) or a^+ (Stokes, forbidden for lowest fundamental transition).

In 3D bulk material, the primary contributions come from the $q \approx 0$ phonons. In 2D SQW, the primary contributions still come from the smallest q values for $L_z > 50\text{\AA}$, or $q_x \approx q_y \approx 0$, $q_z = \pi/L_z$ (H. Qiang *et al*, 1992c). The surface/interface phonon contribution is smaller than the bulk like LO phonon for $L_z > 50\text{\AA}$ as shown by both the experimental results of K. T. Tsen *et al* (1991) and the theoretical results of M. A. Stroscio *et al* (1991). The phonon confinement restricts the available q_z values to $q_z = m\pi/L_z$ ($m=1,2,3,\dots$) so that the smallest q_z is π/L_z instead of zero. In Eqs. (5.5)-(5.7), the possible L_z dependence of Γ_{ep} may come from $1/V$, $1/q_z^2$, and M_{fi} . The quantitative dependence of M_{fi} relies on the wavefunction details of both electrons (excitons) and confined phonons. This complicated theoretical approach is still in progress, but M_{fi} change is probably smaller than the other two terms. If we neglect the

change of M_{fi} , the L_z dependence of the Γ_{ep} can be written as:

$$\Gamma_f^i \propto \frac{1}{V} \times \frac{1}{q_{\text{min}}^2} \propto \frac{1}{L_x L_y L_z} \times \frac{1}{(\frac{\pi}{L_z})^2} \propto L_z \quad (5.8)$$

Therefore,

$$\Gamma_{\text{ep}}^i \propto L_z \quad (5.9)$$

This clearly shows the experimentally observed linear dependence of Γ_{ep} (see Fig. 27), and implies that the term M_{fi} is indeed a much slower varying function of L_z . The contributions from $m > 1$ phonons are much smaller, since the coefficient of Γ_f^i is proportional to the inverse square of q_z , or m^{-2} . The success of this theoretical scaling argument suggests that the reduction origin of the electron (exciton)-phonon interaction is the phonon confinement [$\min(q_z) = \pi/L_z$] partially compensated by the phase space density [$\propto (1/V)$] factor.

It should be pointed out that although we have used infinite well model in writing down the quantized q_z value, the result of this scaling argument is still valid to the other more rigorous models such as the microscopic model of K. Huang and B. Zhu (1988a, 1988b).

There are other experimental evidences in support of this argument. Work on group IV material system Ge/SiGe showed no appreciable changes on Γ_{ep} due to L_z (F.

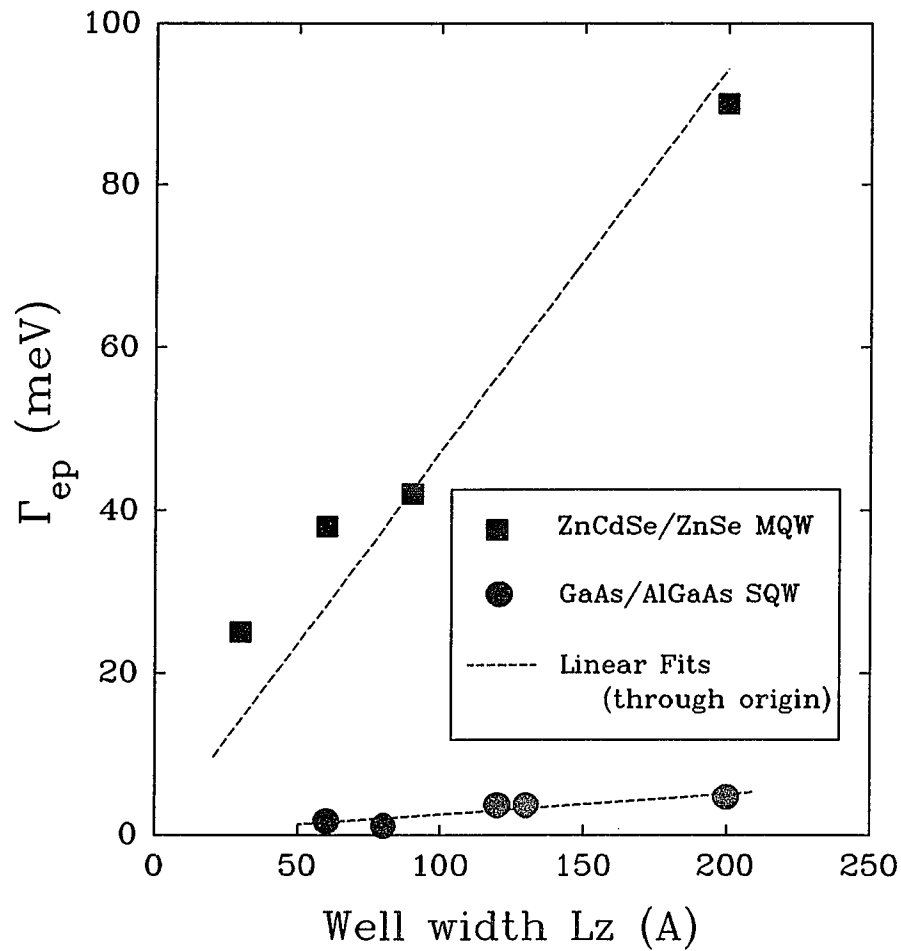


FIG. 28 Γ_{ep} of GaAs/AlGaAs SQWs (solid circles) and $\text{Cd}_x\text{Zn}_{1-x}\text{Se}/\text{ZnSe}$ MQWs (solid squares, Pelekanos *et al*, 1992) of several different well width L_z .

H. Pollak, 1992). On the other hand independent works on group II-VI material systems such as $\text{Cd}_x\text{Zn}_{1-x}\text{Se}/\text{ZnSe}$ ($x=0.25-0.3$) QWs by N. T. Pelekanos *et al* (1992) and $\text{Cd}_{0.33}\text{Zn}_{0.67}\text{Te}/\text{ZnTe}$ QWs by J. P. Doran *et al* (1992) reported much stronger Γ_{ep} reduction. All these results show strong correlation between the reduction of electron (exciton)-phonon interaction with the material polar nature, i.e., its Frohlich interaction origin.

Table IV Experimental values of Γ_{ep} of GaAs/AlGaAs SQWs and CdZnSe/ZnSe MQWs with varying well width L_z .

GaAs/AlGaAs SQWs		CdZnSe/ZnSe MQWs	
L_z (Å)	Γ_{ep} (meV)	L_z (Å)	Γ_{ep} (meV)
60	1.7 ± 0.9	200	90
80	1.1 ± 0.9	90	42
120	3.7 ± 0.6	60	38
130	3.7 ± 0.6	30	25
200	4.7 ± 0.6		
bulk GaAs	20 ± 1	bulk ZnSe	≥ 60

The experimental results of Γ_{ep} of various L_z obtained by N. Pelekanos *et al* (1992) from the temperature dependent absorption measurements on ZnCdSe/ZnSe MQWs are duplicated in Table IV. The value of ZnSe is not quite appropriate for the

comparison purpose here since it is the barrier material instead of the well material. A reduction of Γ_{ep} is also observed. The dependence of Γ_{ep} on the L_z is much clear if we plot them out in Fig. 28 (solid squares). It can be seen that their data is in strong support of the Eq. (5.9). For comparison purpose, our data on III-V material is displayed on the same figure as solid circles. Because of the different polar nature, it is evident that II-VI material shows stronger L_z dependence than the III-V material. We estimated the ratio of $E_{LO}(1/\epsilon_\infty - 1/\epsilon_0)$ for the well materials of the two material systems based on experimental values of E_{LO} , ϵ_∞ , and ϵ_0 . The obtained value of 3 is smaller than the experimental observations of about 20. Clearly more detailed work is needed in order to understand the quantitative behavior in different material systems. One possible explanation (although may not be the only one) for this discrepancy is, as the authors suggested, due to much stronger exciton confinement in II-VI material systems to such

an extent that the exciton binding energy in narrower wells may be larger than the LO phonon energy, which effectively reduces the number of available scattering states $|f\rangle$ [see Eq. (5.5)]. Some more work on this system of the L_z between 90Å and 200Å is needed to clearly establish the role of this contribution, by examining whether the Γ_{ep} will jump abruptly or vary gradually through this region.

5.3.4 Suppression of Exciton-Phonon Interaction by Interface AlAs Monolayers (GaAs/AlGaAs SQW)

In the preceeding section, we see that the electron (exciton)-phonon interaction is reduced as the dimensionality (L_z) of the system is reduced. Besides the linear reduction due to L_z , other modifications on the semiconductor microstructures can also bring about changes on the Γ_{ep} . For example, in the growth of GaAs/AlGaAs QWs, insertion of several mono layers (MLs) of AlAs at interfaces has found to produce samples with narrower features at room temperature. This has proven to be an effective way from material growth experience. Its mechanism has not been understood before and these AlAs mono layers are called "smoothing" layers in a perception that they might help forming interfaces of better quality.

We have carried out a systematic study on the effects of these AlAs MLs. Our experimental results show that on the contrary they probably make the interfaces even worse, which is evident from the broader linewidth at very low temperature. The true mechanism behind is the suppressed electron (exciton)-phonon interaction so that the

thermal broadening difference can be more than a compensation at room temperature. The detailed work in this area can improve our knowledge on the electron (exciton)-phonon interaction in reduced dimensional systems and may suggest more effective ways in sample fabrication stage.

The GaAs/AlGaAs SQW samples were grown by GEN-II MBE at University of Glasgow. Four samples of the same well width (120 Å) were grown at identical conditions with varying AlAs ML thickness at either interface. The attempted AlAs interface layer thicknesses are 0, 3, 6, and 9 ML.

Again temperature dependence of the line-width of fundamental 11H QW transition is studied by PR technique. The same data analysis procedure was adapted as discussed in the preceeding section. Obtained Γ_0 (open circles) and Γ_{ep} (solid circles) for the four different samples are

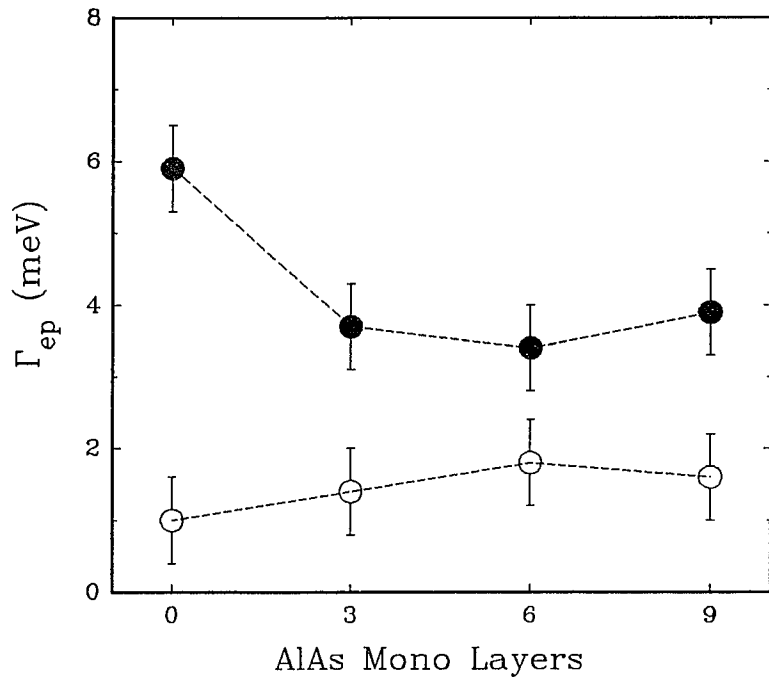


FIG. 29 Experimental values of Γ_0 (open circles) and Γ_{ep} (solid circles) of a series of GaAs/AlGaAs SQWs with varying AlAs interface layer thickness.

displayed in Fig. 29 as a function of AlAs interface layer thickness. It can be seen that Γ_0 of 0 ML sample is the best among them, indicating no evidence of improved interface quality associated with AlAs interface layers. The Γ_{ep} of 3, 6, and 9 ML samples are found within the experimental error bars, but Γ_{ep} of 0 ML puts itself higher away from the rest. It is clear that AlAs ML plays a role in reducing the Γ_{ep} and this effect is saturated above 3 ML thickness.

This experimental observation may find its root in the matrix element M_{fi} of Eqs. (5.5)-(5.7), which needs and currently under further investigations.

5.4 Summary

Temperature change will bring about changes on various electronic properties. Some experimental results of this work are summarized here:

- The modulation spectroscopy line shape function could be temperature dependent, which has been reported evolving from FDLL to FDGL in going below 80K to higher temperatures on GaAs/AlGaAs MQW. Our work on bulk GaAs E_0 exciton, an InGaAs/GaAs SQW, and GaAs/AlGaAs SQWs shows that the FDGL is also possible at low temperatures. Since in most cases there is only small linewidth change around 80K, the continuation of the same line shape function at low temperatures is a more natural choice. The result justifies the sum of FDGL and FDLL (below 80K in some instances) functions as an adequate set for exciton

features but shows that caution must be taken in associating the absence of pronounced "wings" to a FDLL.

- The temperature dependence of the fundamental exciton transition energy is well described by Varshni Eq. (5.1). Their quantitative behavior generally follows that of the well material.
- The improved resolution at low temperatures of various optical spectroscopy is because of the reduced linewidth. Its quantitative behavior can be well described by Eq. (5.3) which interprets the temperature dependence as mainly due to LO phonon populations. The quantitative dependence is different between the bulk material and semiconductor microstructures.
- The temperature dependence of linewidth (thermal broadening) offers a convenient way to explore the electron (exciton)-phonon interaction. Our study on a series of GaAs/AlGaAs SQWs ($60\text{\AA} < L_z < 200\text{\AA}$) shows a linear dependence of the coupling constant Γ_{ep} on the well width L_z . In another word, the carrier phonon interaction will be reduced in reduced dimensional systems. The linear dependence on L_z can be understood by a scaling argument of Frohlich interaction without touching the details of the scattering matrix element M_{fi} [see Eqs. (5.5)-(5.9)].

- The electron (exciton)-phonon interaction depends on the system dimensionality. It may as well be changed by other means. For example, our preliminary result has shown that the insertion of several MLs of AlAs at QW interface may effectively reduce this coupling.

Chapter 6. Electric Field Effect

6.1 Introduction

If an atom is placed in an electric field, the atomic energy levels will be shifted and certain degeneracies will be removed. This Stark effect has a characteristic energy of eFa . However, it is very difficult to observe the Stark effect in bulk semiconductors because the excitons are very easily ionized. Instead the Franz-Keldysh oscillation (FKO) associated with the band edge is usually observed. The new properties of semiconductor microstructures, such as extra confinement and interwell coupling, makes it possible to study the Stark effect as well as various other effects of electric field. It is possible to study a particular effect by choosing the structure parameters. Thus, studies of the effects of electric fields are very important in the understanding of many fundamental properties of semiconductor microstructures such as the quantum confined Stark effect (QCSE) in SQWs, interwell coupling and decoupling in coupled double quantum wells (CDQW), and Wannier-Stark quantization in SLs. The Stark effect will be much enhanced in a quantum confined system because the electron and hole pairs are more difficult to be dissociated. The QCSE has been shown to persist with considerable oscillator strength in a field over 100kV/cm in SQWs. We show the results of our theoretical model on a typical GaAs/AlGaAs SQW under various electric field bias in section 6.3.1.

Our work on a symmetrically coupled GaAs/AlGaAs double quantum well

structure demonstrates some interesting phenomena as compared to the bulk materials. We observed (a) strong resonance coupling at $F=0$, (b) linear Stark shift due to decoupling and resonance coupling of higher transitions at resonance field at $F>0$, and (c) QCSE and field induced broadening at excessively large fields $F\gg 0$. These results will be discussed in section 6.3.2.

In section 6.3.3, works on HEMT structures will be presented. It is another important and interesting device structure. The modulation spectroscopy has shown some distinctive advantages in characterizing these structures.

6.2 Experimental Setup

There are many ways of achieving electric field inside a semiconductor microstructure. For example, built-in electric field can be generated across certain layers simply by varying the doping level during the sample growth, either deliberately or not. The electric field thus obtained will be maintained in a free standing sample. HEMT structure is a typical example of this kind.

Uniaxial stress can also generate electric field in polar materials such as GaAs due to piezoelectric effect if the stress direction is not along the high symmetry (001) axis. This phenomenon will be discussed in more detail in chapter 7 when we discuss the uniaxial stress effects.

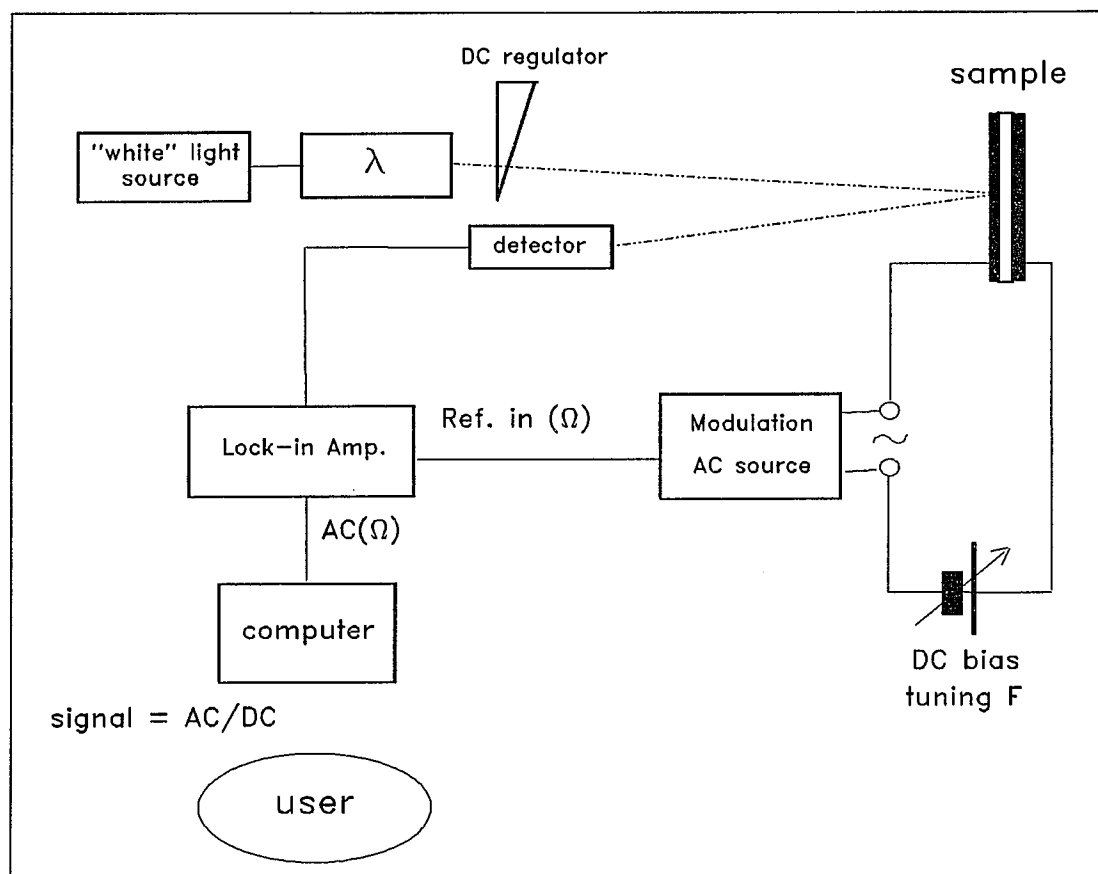


FIG. 30 Schematic diagram of an ER setup.

The more direct control of electric field is by evaporating electrodes on to the sample and then tuning the electrical voltage across them. Since in this situation the electrodes are readily available, the ER experiment is a good choice where the modulation *ac* voltage and the field tuning *dc* voltage can be easily superimposed on to the very same pair of electrodes. A typical ER set up is schematically shown in Fig. 30. The work of CDQW in section 6.3.2 is a typical example of this situation.

6.3 Experimental Results

6.3.1 Quantum Confined Stark Effect in SQW Structure (GaAs/AlGaAs SQW)

In QWs, the Stark effect can be more easily observed as compared to the bulk semiconductor materials. The oscillator can persist considerable strength up to very high electric field since the electron and hole pairs are more difficult to dissociate. The Stark shift is also larger because the characteristic energy $eFa = eFL_z$ is bigger. A theoretical calculation of a 100Å GaAs/Al_{0.3}Ga_{0.7}As SQW is shown here as an example to demonstrate the QCSE. The details of this theoretical calculation method have been discussed in Chapter 4.

Shown in Fig. 31(a) is the calculated exciton transition energies of 11H, 12H, and 11L features of a 100Å GaAs/Al_{0.3}Ga_{0.7}As SQW under various electric fields. Exciton binding energy has been taken into account from a variational approach. All the features undergo dramatic red shift (QCSE). The 11H and 11L have about the same amount of field induced shifts. The oscillator strength is usually estimated by the square of wavefunction overlap integral. The calculated values of 11H and 12H features are shown as dashed lines in Fig. 31(b). As the field increases, the 11H feature decreases monotonically because the electron and hole move to the opposite direction. On the other hand, the 12H feature increases up to 100kV/cm because of the breakdown of selection rules, and decreases afterwards due to increased field induced tunneling probability. A more rigorous estimate of the exciton strength must take into account of the exciton binding effect. Shown in Fig. 31(b) as solid lines are the calculated exciton

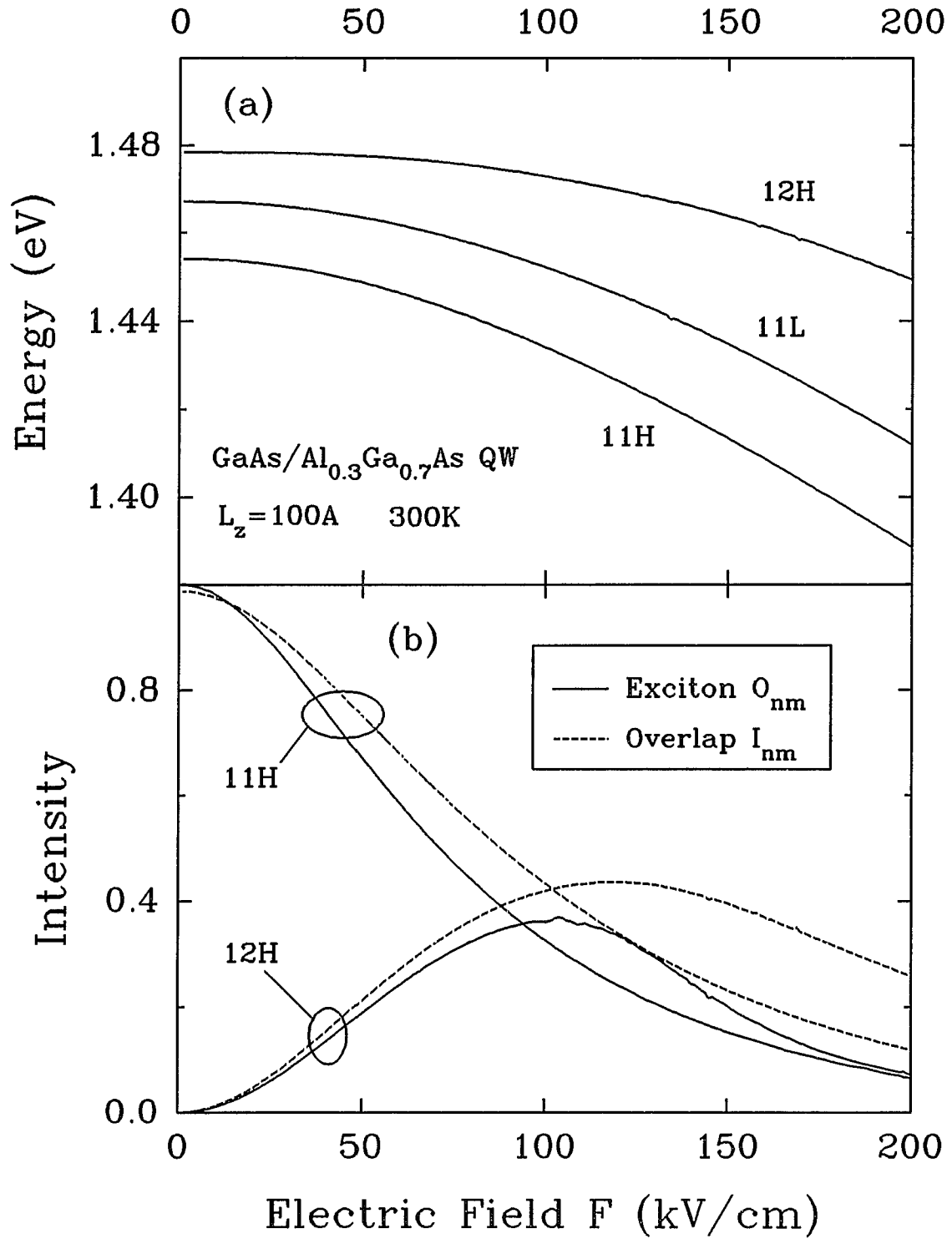


FIG. 31 Calculated electric field dependence of (a) transition energies and (b) exciton intensities (solid lines) and wavefunction overlap integral (dashed lines) of a GaAs/AlGaAs SQW.

oscillator strength normalized to the 11H feature at $F=0$. The oscillator strength O_{nm} is given by:

$$O_{nm} \propto |P_{cv} \times I_{nm} \times \phi_{nm}(0)|^2 \quad (6.1)$$

where,

$$\begin{aligned} P_{cv} &= \langle c | p | v \rangle \\ I_{nm} &= \langle f_n^c | f_m^v \rangle \end{aligned} \quad (6.2)$$

where $|c\rangle$ and $|v\rangle$ are the Bloch wavefunctions of conduction and valence bands, respectively. The ratio of P_{cv} between HH and LH features is 3:1. The envelop wavefunction overlap integral I_{nm} is the dominant source of the field dependence of oscillator strength, since the change of exciton wavefunction $\phi_{nm}(0)$ is smaller. This is evident in Fig. 31(b) if we compare the solid and dashed lines.

In conclusion, in SQWs, there are two major characteristic behavior of QCSE. As the electric field along the growth direction increases, (a) the oscillator energy positions are redshifted to lower energy side and (b) the oscillator strength of the "allowed" transitions such as 11H decreases while the "forbidden" transitions such as 12H becomes more important.

6.3.2 Enhanced Stark Effect in CDQW Structure (GaAs/AlGaAs CDQW)

Recently, coupled quantum well systems have attracted increasing attention because of both their basic and applied properties. Coupling effects in semiconductor

SLs or MQW structures in electric fields cause significant phenomena in the optical properties such as Wannier-Stark localization (P. Voison, 1988) and quantized level mixing. The application of coupling effects to optoelectronic devices could bring about fruitful results such as the QCSE. For example, there has been considerable effort to further enhance this effect, in particular to increase the size of the energy shift for a given applied field. To achieve this goal a coupled double quantum well structure has been proposed. In an isolated SQW, transitions between the ground state of the electron in the conduction band and the ground state of the heavy and light holes in the valence band give rise to a doublet in the absorption spectra related to the ground state heavy- and light- hole excitons. When two SQWs are brought into close proximity, wave-functions of the confined electrons and holes can overlap, leading to mixing and split levels in the conduction and valence bands. Since each of the original levels is doubled, a maximum of eight transitions is allowed out of original 11H and 11L two transitions. If the two SQWs are identical and unperturbed, the split levels have well defined symmetry. Selection rules dictate that the transitions are allowed only between levels of the same symmetry which results in only four allowed features. Application of an electric field creates a perturbation which decouples the wells leading to spatially indirect (inter-well) structures which show significant shifts in energy. A systematic investigation of the coupled double quantum well structure is thus important for a better understanding of the basic properties of more complex structures such as SLs and MQWs. In addition, it has significant device aspects.

While optical studies of symmetrically and asymmetrically CDQWs have been reported using photoluminescence (C. Jagannath *et al*, 1988), photoluminescence excitation spectroscopy (Y. J. Chen *et al*, 1987; J. Lee *et al*, 1989; S. R. Andrews *et al*, 1988; C. Jagannath *et al*, 1988), photocurrent spectroscopy and reflectivity (P. Bonnel *et al*, 1990), little work has been done using modulation spectroscopy (C. Cacciatore *et al*, 1989; O. J. Glembocki *et al*, 1991), in spite of its proven utility in providing information about semiconductor microstructures (see for example F. Pollak and Glembocki, 1988 and references therein). PR (C. Jagannath *et al*, 1988) and ER (C. Cacciatore *et al*, 1989) work on CDQWs at 300K have utilized the sharp, derivative-like features of electromodulation to study band structure effects, i.e., field induced shifts. However, these works did not perform any detailed line shape fits. Recently Glembocki *et al* (1991) have reported an ER study of asymmetrically coupled GaAs/AlGaAs and InGaAs/GaAs systems in which the details of the line shape were used to evaluate not only energy shifts but also to characterize the resonance of the coupling.

We have carried out a systematic study of the ER spectra at 77K of a GaAs-/Al_{0.23}Ga_{0.77}As symmetric CDQW as a function of external bias (Y. S. Huang *et al*, 1991a). The value of the internal field was directly evaluated from the FKO observed in the spectra of the direct gap of the AlGaAs barrier material (X. Yin *et al*, 1990). A detailed line shape fit was used to not only accurately determine the energies of the various spectral features but also to obtain information about the nature of the modulation mechanism in this structure. The line shape fits also have enabled us to observe features

which were not directly evident in the spectra. The experimental values of the energies are in good agreement with a theoretical calculation based on the resonance method (E. J. Austin and M. Jaros, 1985). At low fields the resonance energy positions were taken from the Breit-Wigner parameterization and exciton binding effects were then estimated using a variational method while at high fields we employed density-of-states maximum positions.

The material used in this study was fabricated by molecular beam epitaxy at the GTE laboratories. The sample was grown on an (001) n^+ -GaAs substrate and consisted of a single pair of GaAs quantum wells ($L_w=6.0\text{nm}$) separated by a $\text{Al}_{0.23}\text{Ga}_{0.77}\text{As}$ barrier ($L_B=2.2\text{nm}$), two 85nm outer undoped $\text{Al}_{0.23}\text{Ga}_{0.77}\text{As}$ barriers and a 20nm p^+ -GaAs cladding layer, all on a n^+ -GaAs buffer. A Ni/Au-Ge/Au metallization, with 3-min 450°C sintering, was employed to obtain an Ohmic contact to the n^+ substrate while an annular ring by Au-5 at. % Zn metallization provided a near-Ohmic contact to the p^+ -GaAs cladding layer. Thus the CDQW portion of the sample was in the insulating region of a p-i-n configuration.

The experiment was performed at 77K. The ER apparatus has been described previously (see Fig. 30). The *ac* modulation was a 880Hz sine wave with a peak-to-peak amplitude of 0.1V, which corresponded to an electric field value of $5.5 \times 10^3 \text{V/cm}$. Various values of the *dc* bias voltage were employed.

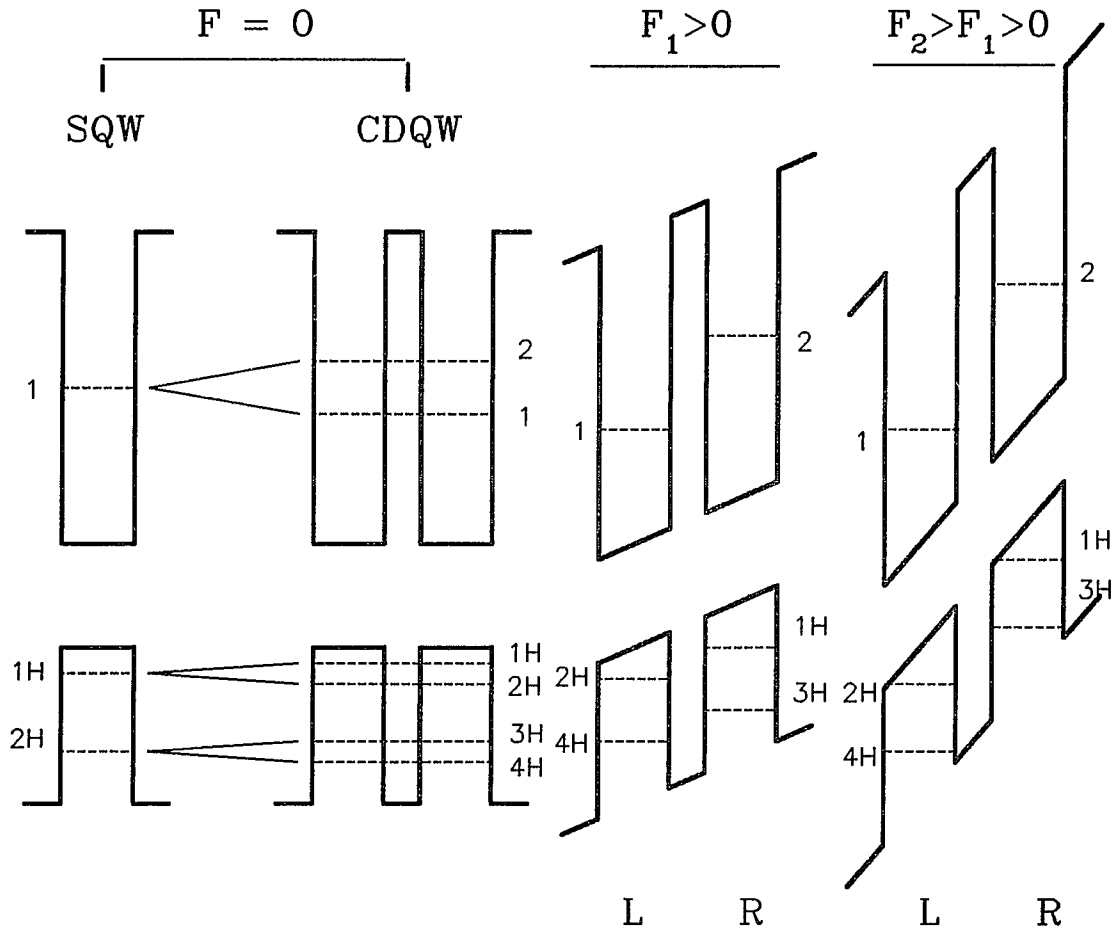


FIG. 32 Schematic band diagram of a SQW, a symmetrically CDQW of $F=0$, and in the presence of electric field $F_2 > F_1$. For simplicity only show (a) HH states and (b) off-resonance for $F > 0$.

Shown in Fig. 32 is a schematic representation of the energy levels of a SQW (left), a symmetric CDQW under flatband conditions ($F=0$) and in the presence of intermediate (F_1) and large (F_2) electric fields. For simplicity we show only the heavy-hole (H) valence states. In the SQW there exists a series of discrete levels for both electrons and holes due to the square well potential. In the symmetric CDQW the barrier is narrow enough so that the wavefunctions of the electronic states in the conduction (or valence) bands in the adjacent wells overlap and therefore split into symmetric and anti-

symmetric components. In the absence of external perturbations (i.e., flat band condition) the state symmetries are well defined and only symmetry allowed transitions can occur. We keep using the notations $mnH(L)$ as in SQWs. The levels m/n here are assigned as follows: the pair of numbers (1,2) designates the levels which originate in the ground states of the conduction/valence bands, the pair (3,4) corresponds to the first excited states, etc. The odd and even numbers are the symmetric and anti-symmetric states of the CDQW, respectively, at $F=0$. For the flatband conditions and for infinite wells for the electron/holes only the so-called "symmetry"-allowed transitions with $m=n$ should be observed. However, for finite wells "parity"-allowed transitions with $m=n\pm 2, \pm 4, \dots$ are also possible, although they are probably weak. In the former case there is a simple relationship between the number of nodes of the wavefunction in the well and the energy of that state which leads to the $m=n$ "symmetry"-allowed selection rule. For latter situation nodes may appear in the barrier and hence the parities of the states with respect to the center of the well no longer alternate. In the presence of an electric field ($F>0$) the wavefunction symmetries are distorted, the selection rules are relaxed and all transitions become possible. In this case $m=n$ and $m\neq n$ correspond to "interwell-like" (spatially indirect) and "intrawell-like" (spatially direct) transitions, respectively. It should be noted that even for $F>0$ there is still some wavefunction overlap between adjacent wells. For example, in Fig. 32 for $F>0$ the $n=1$ conduction state in the left well has some penetration into the right well. However, for clarity this is not shown.

Shown in Fig. 33 by the solid lines are the experimental ER spectra for external bias voltages (V_b) of +1.5, +1.0, +0.5, 0, -1.5 and -3.8 V in the photon energy range 1.4 - 2.4 eV. The features below 1.7 eV correspond to transitions in the GaAs CDQW. For $V_b = +1.5$ V this portion of the spectrum has a large number of resonances while for reverse bias the data becomes much simpler. Only two peaks are observed for $V_b = -1.5$ V, while for $V_b =$

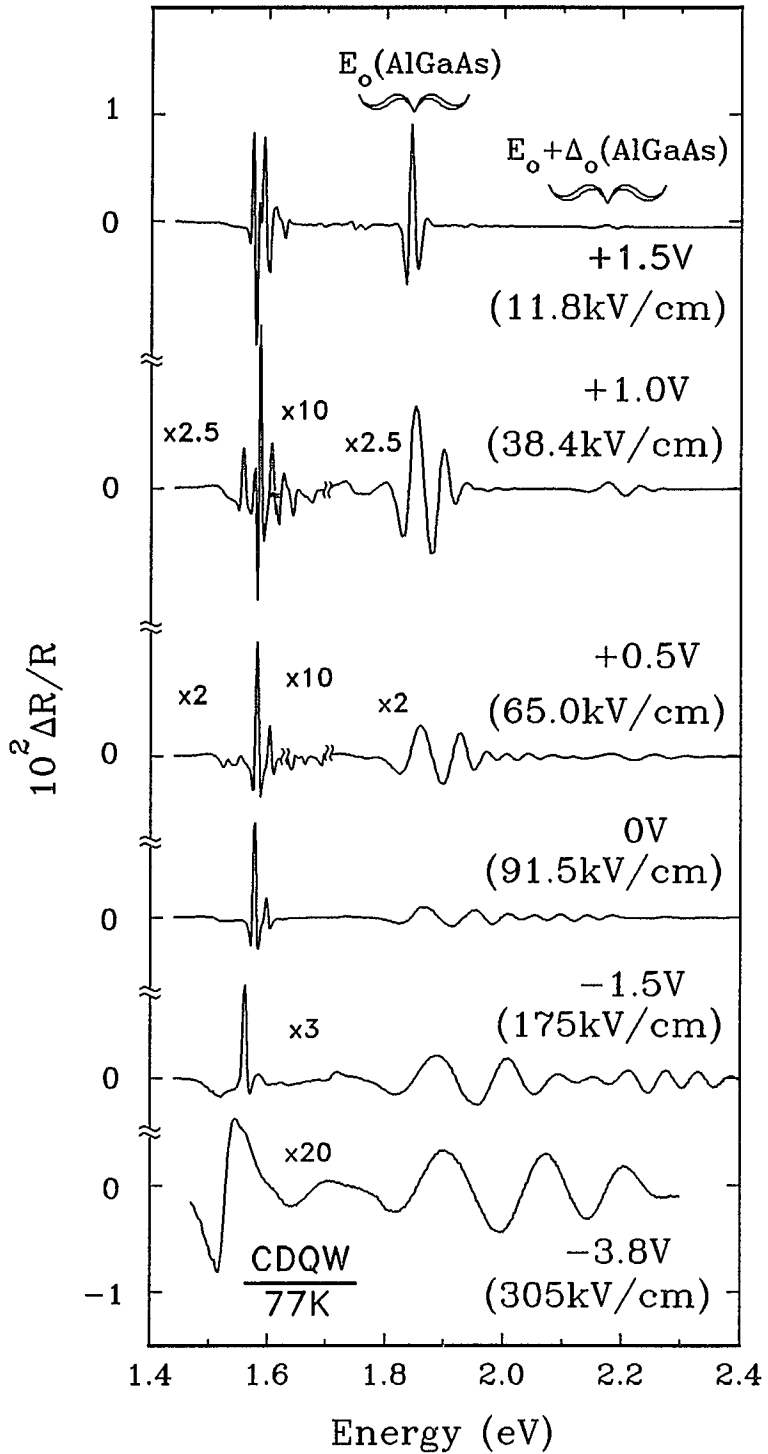


FIG. 33 ER spectra of a GaAs/AlGaAs CDQW structure at 77K for various external biases (V_b). Also displayed are the electric fields as deduced from the FKO of $E_0(\text{AlGaAs})$.

= -3.8 V they have become fairly broad. Above 1.8 eV the spectra are due to the direct transition (E_0) and spin-orbit split component ($E_0 + \Delta_0$) of the $\text{Al}_{0.23}\text{Ga}_{0.77}\text{As}$ cladding layers. These latter features exhibit FKO which have enabled us to directly and accurately determine F in the insulating region of the sample which contains the CDQWs. For example, for $V_b = +1.5$ V the field is $F = 11.8$ kV/cm and so the sample is almost at flat band. On the other hand for $V_b = 0$ there is already a large built-in field of $F = 91.5$ kV/cm as evidenced by the large number of FKO. From the position of $E_0 = 1.839$ eV we have deduced an Al composition of $x = 0.23$ (D. E. Aspnes *et al*, 1986). For spectra near flatband condition some small features are observed at about 1.75eV. These are due to transitions such as 31H and 31L. They quickly disappear with increasing field.

Displayed
by the solid lines
in Figs. 34-37 are
the experimental
ER data in the
region of the GaAs
CDQWs (1.48-
1.71eV) for $V_b =$
+1.5, +0.5, -1.5,
and -3.8 V, re-

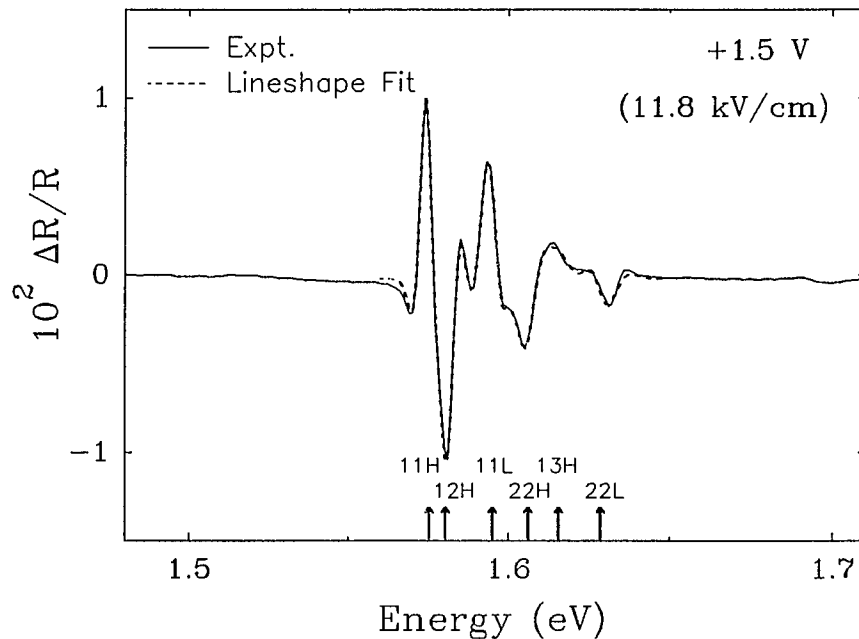


FIG. 34 ER spectra at 77K originating from the CDQW for $V_b = 1.5$ V. The obtained values of the various transition energies are designated by arrows.

spectively. The dashed lines are least-squares fits to equation (Y. S. Huang *et al*, 1991a):

$$\Delta \frac{R}{R} = \sum_j C_j \left[\sin \theta_j f_x^{(1)}(y_j) + \cos \theta_j f_x^{(2)}(y_j) \right] \quad (6.3)$$

$$y_j = (E - E_j) / \Gamma_j$$

Where C_j is the amplitude of j th component, phenomenological phase angle θ_j represents the mixing of real and imaginary parts, and $f_x^{(1)}$ and $f_x^{(2)}$ are the two FDGL functions [see Eq. (3.12)].

In Fig. 34, which corresponds to almost flatband, six oscillators ($j=6$) have been resolved. They are designated 11H, 12H, 11L,

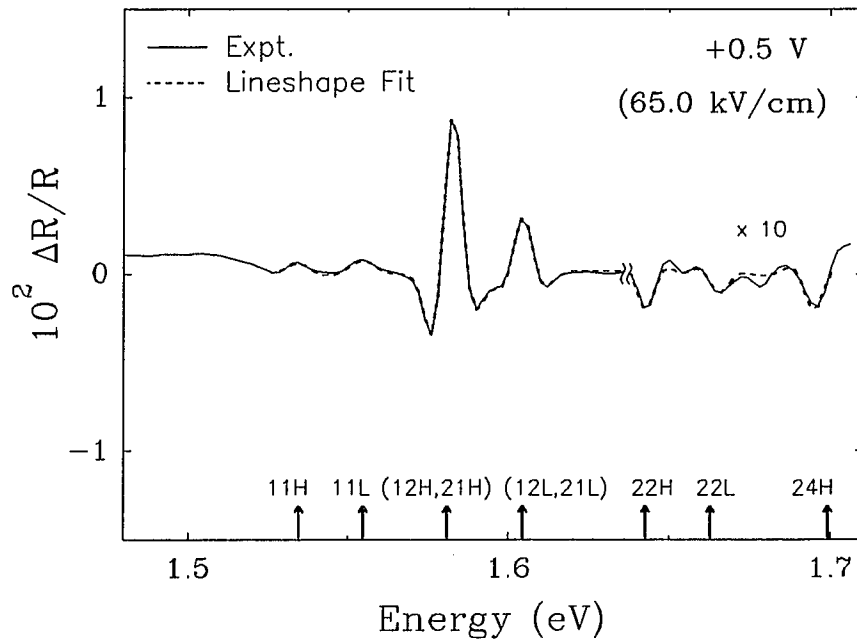


FIG. 35 ER spectra at 77K originating from the CDQW for $V_b=0.5V$. The obtained values of the various transition energies are designated by arrows.

for this arrange-

ment will be discussed below. Their energies are denoted by arrows at the bottom of the figure. Although it appears that there is only one transition in the region of the large,

lowest feature (≈ 1.575 eV), the detailed lineshape fit reveals the presence of two resonances, 11H and 12H. The positive lobe corresponds to the former while the negative lobe originates from the latter. The spectral features with $m=n$ are "symmetry"-allowed while 12H and 13H are "symmetry"-forbidden. Although 13H is "parity"-allowed, the appearance of 12H is probably due to the presence of the small electric field.

As shown in Fig. 35, increasing the electric field ($V_b = +0.5$ V) causes a red (blue) shift of the 11H and 11L (22H and 22L) transitions

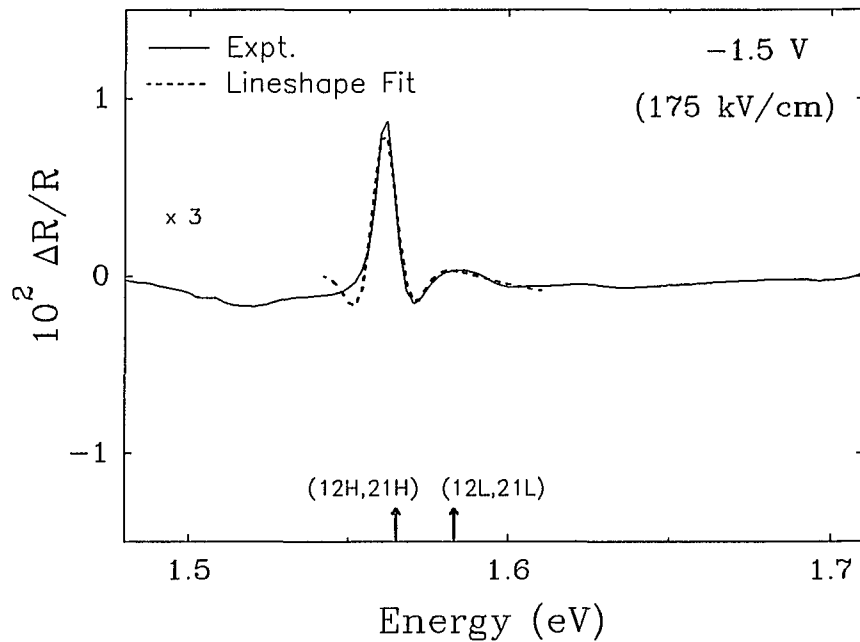


FIG. 36 ER spectra at 77K originating from the CDQW for $V_b = -1.5$ V. The obtained values of the various transition energies are designated by arrows.

intensities. The

strongest spectral structure corresponds to the "symmetry"-forbidden (12H, 21H) intra-well transitions (see Fig. 32). Also the 24H transition at about 1.699 eV becomes visible.

The spectrum for -1.5V (Fig.5) is quite simple in relation to the cases for the lower electric fields. It consists of only the two features (12H,21H)

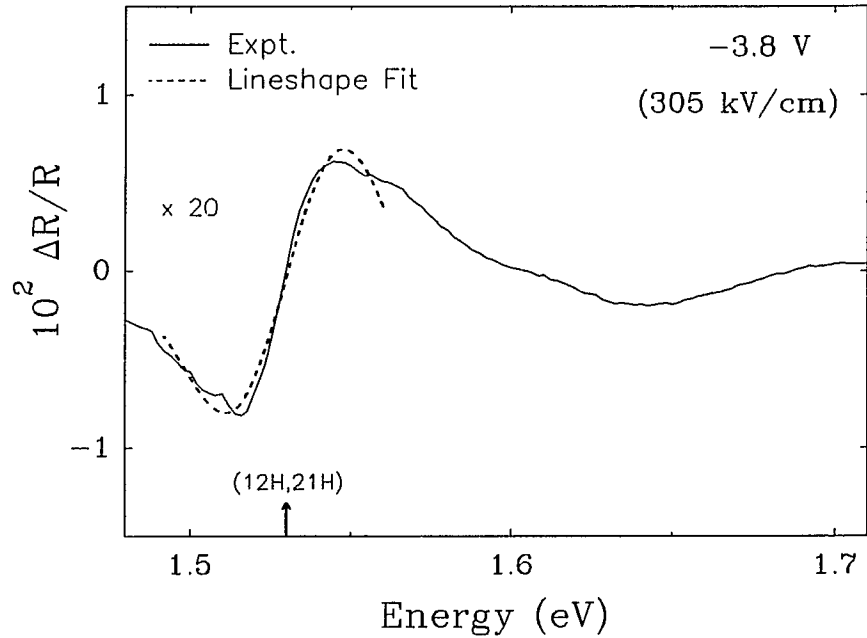


FIG. 37 ER spectra at 77K originating from the CDQW for $V_b = -3.8\text{V}$. The obtained values of the various transition energies are designated by arrows.

bias ($V_b = -3.8\text{V}$)

these two peaks become quite broad due to the field induced tunneling effect (see Fig. 37). Although this line shape has been fit to Eq. (3.12), (6.3) with $j=1$ for (12H,21H) to estimate its resonance position and phase angle θ , at this large field other modulation mechanisms come into play and so that the true meaning of θ is no longer that of Eq. (3.12), (6.3). Even though Eq. (3.12), (6.3) may not be rigorously correct at high fields the obtained energies are still accurate. It has been demonstrated that the energy of a resonance is relatively insensitive to the details of the line shape fit (F. H. Pollak and O. J. Glembocki, 1988; O. J. Glembocki and B. V. Shanabrook, 1989). However, the determination of other factors such as Γ and θ are much more dependent on the particular line shape function that is employed.

The results of Figs. 34-37 can be understood on the following basis. At flatband ($F=0$) the spectrum should consist mainly of the "symmetry"-allowed transitions ($m=n$) such as 11H, 11L, 22H and 22L. The application of a field tilts the potential and produces a redistribution of the wavefunctions. The low energy coupled states of the valence band (1H,1L) concentrate mostly in the right well (designated R in Fig. 32) while the low-energy coupled level of the conduction band resides primarily in the left well (marked L in Fig. 32). The reverse is true for the high-energy coupled levels (anti-symmetric states under flat band). For $F>0$ intra-well transitions in either the L (12H and 12L) or R (21H or 21L) QWs experience the regular QCSE (D. A. B. Miller *et al*, 1985) and are only weakly affected by the coupling since the energy shifts of the electron and hole states nearly cancel each other. In fact once the wells are decoupled, 12H (12L) and 21H(21L) are almost degenerate in energy. On the other hand, the energies of interwell-like transitions undergo rapid Stark shift decreases (11H and 11L) or increases (22H and 22L) with increasing F since these transitions couple electron and hole states either moving toward or away from each other. Thus, symmetry-allowed transitions ($m=n$) under the flatband situation become interwell-like transitions under an applied field while $m \neq n$ transitions become intrawell-like under sufficiently large fields. The wavefunction overlap of electron and hole states localized in different wells is substantially reduced. In this case, interwell-like transitions (11H, 11L, 22H, 22L) are expected to weaken while intrawell-like features [(12H,21H) and (12L,21L)] approach those observed in a SQW. Thus, as shown in Fig. 33 for $V_b=0V$, $-1.5V$ and $-3.8V$ only two peaks corresponding to (12H,21H) and (12L,21L) are seen in the spectra

originating in the CDQW. Further application of large fields results in a significant red shift (QCSE) and broadening of the feature, as reported for a SQW (D. A. B. Miller *et al*, 1985).

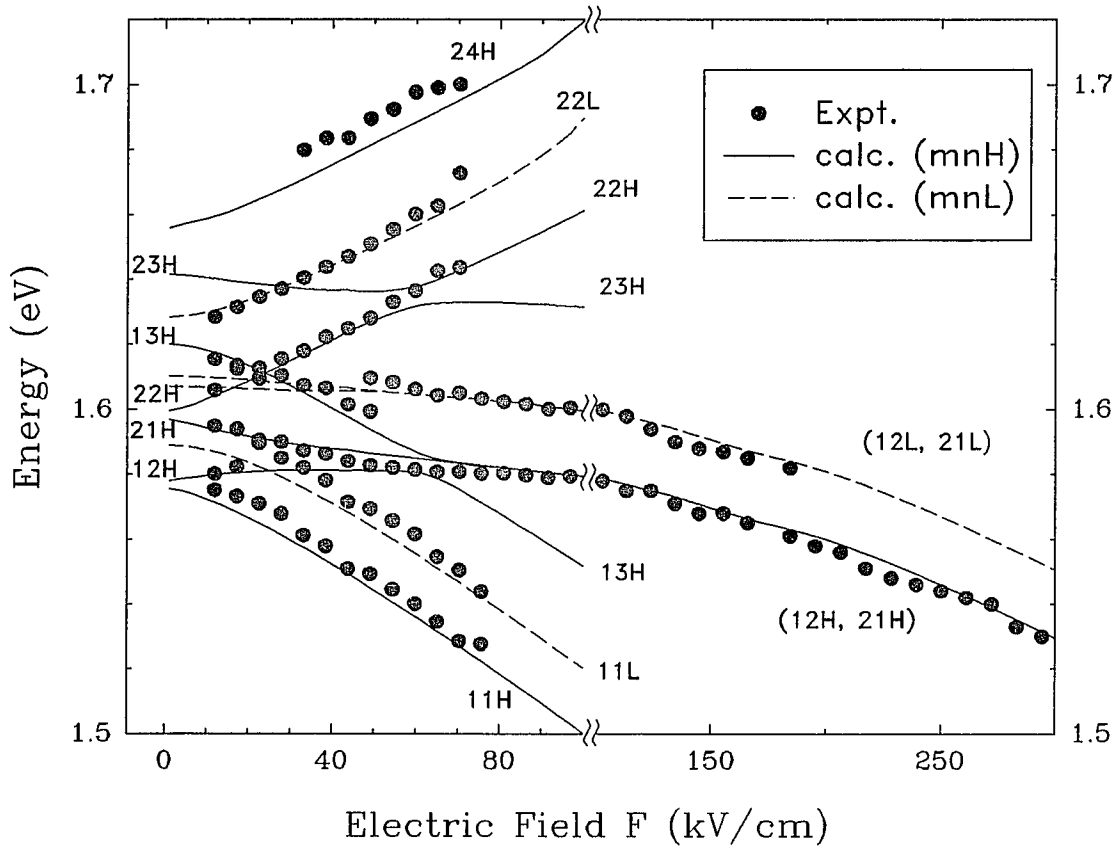


FIG. 38 Various experimental transition energies of the CDQW as a function of electric field. The solid (dashed) lines are the theoretical values for the mnH(L) transitions.

In order to more quantitatively interpret our data we have calculated the various energy levels in an electric field using resonance methods (E. J. Austin and M. Jaros, 1985), in particular the resonance energy positions from the Breit-Wigner parametrization and positions of density-of-states maximum (see Appendix A). The former approach,

which takes into account of exciton binding effects by a variational method, was employed at low fields. However, at high fields the more physically meaningful property is the field dependence of the density-of-states and in this case the latter technique was used. In the calculations we employed the parameters L_w and L_b from the growth condition and a conduction to valence band offset ratio of 65:35. Plotted in Fig. 38 by the solid circles are the experimental energies of the various CDQW features (1.5-1.72 eV) as obtained from the line shape fit while the theoretical energies for the mnH and mnL transitions are denoted by solid and dashed lines, respectively. The comparison of the experiment and theory, including electric field dependence has been used to identify the origins of the various features, particularly at low field. In general there is very good agreement between experiment and theory. The 11H, 11L, 22H, 22L "symmetry"-allowed transitions at flatband become interwell-like for $F > 0$ and experience a linear Stark shift with slope $\approx e(L_w + L_b)$. For $F > 70 \text{ kV/cm}$ the 12H(12L) and 21H(21L) features have become almost degenerate since the wells are now completely decoupled due to the fact that the Stark energy $[e(L_w + L_b)F]$ is now much greater than the characteristic coupling energy. The latter can be estimated from the zero field separation between 21L and 11L ($\approx 20 \text{ meV}$).

The detailed line shape fit of Eq. (3.12), (6.3) to the experimental ER spectra produces not only accurate energy values of the various transitions but also yields other important information. For example, the line shape fit of Fig. 35 reveals that all 7 features have predominantly a $f_x^{(1)}$ profile. This observation implies $\cos\theta_j \approx 0$, in

agreement with the equation $\theta = [4\pi n(\lambda) T \cos \theta_r] / \lambda$ proposed by Thorn *et al* (1987) (see Y. S. Huang *et al*, 1991a). The phases of these spectral resonance fall into two categories. The $j=1-4$ [11H, 11L, (12H, 21H), (12L, 21L)] features have a positive lobe while for $j=5-7$ [22H, 22L and 24H] the phase is reversed. This reversal in the sign is due to the gap modulation response factor dE_j/dF (see Chapter 3). As shown in Fig. 38, for $F \geq 60$ kV/cm the field dependence of the energies of the observed transitions (i.e., $dE_{x,j}/dF$) do indeed fall into two categories, i.e., 11H, 11L, (12H, 21H) and (12L, 21L) have opposite slope in relation to 22H, 22L, and 24H.

The field dependence of 12H is of particular interest. For $F < 50$ kV/cm this transition undergoes a small blue shift due to the quantum well coupling effect while for larger fields a red shift is observed, similar to its SQW counterpart. This change in the movement of the 12H energy with field is also manifest in the phase angle θ_{12H} of the 12H feature. For example, in Fig. 34 the 12H line shape has a negative lobe while in Fig. 4 the phase has reversed, i.e., positive lobe similar to 11H and 11L. Plotted in Fig. 39 is θ_{12H} as a function of field F . At $F \approx 50$ kV/cm $\theta_{12H} \approx \pi$ which results in a change in the sign of $\sin \theta_{12H}$. This corresponds approximately to the field where the motion of 12H changes from a blue to a red shift (see Fig. 38). The dashed line approximately indicates the region where Eq.(7) starts to fail and hence θ_{12H} no longer represents the contribution of only f_x . For $F \geq 200$ kV/cm other modulation mechanisms such as f_r and f_l (see Chapter 3) become important. For instance, comparison of Fig. 36 and Fig. 37 reveals that there is considerable field induced broadening of (12H, 21H).

It should be noted that although the blue shift in the energy of 12H is only a few meV (see Fig. 38) there is a sizeable blue shift of the absorption edge up to about 50-60 kV/cm (see Fig. 33). This is similar to the recent observations of Cacciatore *et al* (GaAs/AlGaAs, 1989) and Gershoni *et al* (InGaAs/InP, 1990) in CDQW systems. This

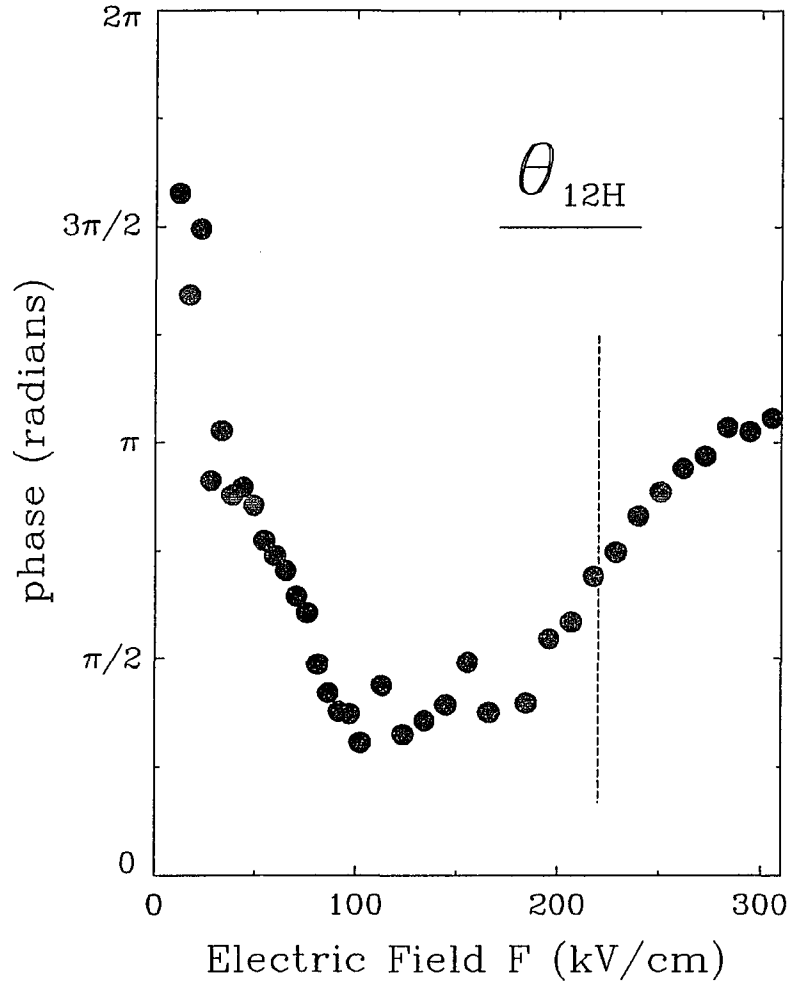


FIG. 39 Phase angle θ_{12H} of the 12H feature as a function of electric field.

latter effect is due primarily to the fact that at $F=0$ the absorption edge is caused by the lowest lying 11H feature, which then red shifts (and loses intensity) with increasing F . This leaves the higher lying 12H peak, which has only a weak field dependence in this range, as the fundamental absorption edge.

In conclusion we have performed a systematic ER study at 77K of the effects of an externally applied electric field in the quantum transitions in a $\text{GaAs}/\text{Al}_{0.23}\text{Ga}_{0.77}\text{As}$

CDQW. The FKO observed in the AlGaAs direct gap region has allowed us to accurately determine F . From a detailed lineshape fit we have been able to evaluate the energy shifts of the various transitions and to obtain information about the modulation mechanism. The high fields achieved in this experiment (300 kV/cm) have enabled us to observe not only the Stark shifts associated with the decoupling of the wells but also a red shift of the (12H,21H) feature due to the QCSE. The energy shifts are in good agreement with a theoretical calculation.

In the next section, I will discuss the work on HEMT structures, where large built-in electric field exists in the MDQW region.

6.3.3 HEMT Structure Investigation Using Modulation Spectroscopy

(AlGaAs/InGaAs/GaAs pseudomorphic HEMT)

Recent advances in the growth of stable strained layer AlGaAs/InGaAs/GaAs quantum wells have produced heterostructure HEMT structures with peak carrier velocities exceeding those of AlGaAs/GaAs alone. In addition, these pseudomorphic structures (a) overcome the problem in AlGaAs/GaAs HEMTs due to the DX center in the AlGaAs (with Al mole fraction over 15%) and (b) make it possible to achieve a large conduction band discontinuity for a given Al composition (H. Morkoc and H. Unlu, 1987; W. J. Schaff *et al*, 1990). Thus in the AlGaAs/InGaAs/GaAs system, large 2DEG carrier concentrations can be achieved while maintain high electron mobilities, alleviating difficulties inherent in the AlGaAs/GaAs approach. These structures hold promise for

device performance up to 400 GHz.

In spite of the proven utility of modulation spectroscopy, particularly electro-modulation, in characterizing semiconductor microstructures (see for example F. H. Pollak, 1991), very little work has been performed on the AlGaAs/InGaAs/GaAs HEMT system. In the EBER investigations by M. H. Herman *et al* (1990) and A. Dodabalapur *et al* (1990) almost no analysis was performed on the optical features associated with the InGaAs region of the samples. Tober *et al* (1989) observed several peaks from the InGaAs MDQW in PR and PzR although no specific features related to the 2DEG were seen.

We report a detailed ER and PR study (Y. Yin *et al*, 1992) of a pseudomorphic $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}/\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ modulation doped HEMT structure in the temperature range $79\text{K} < T < 304\text{K}$ (Y. Yin *et al*, 1992a, 1992b). We have detected several features associated with the InGaAs MDQW portion of the sample, which exhibit an unusual modulation spectroscopy line shape. We have been able to account for these spectral features based on a two dimensional density of states, due to the screening of the excitons by the 2DEG (D. Huang *et al*, 1988; D. S. Chemla *et al*, 1988; G. Livescu *et al*, 1988) and a Fermi level filling factor. From the details of the line shape fit to the lowest lying InGaAs feature we can extract the Fermi level position and hence the density of the 2DEG. By comparing the experimentally obtained energies of the InGaAs intersubband transitions with a theoretical model we can also obtain other important materials

parameters such as the MDQW width (L_z), In composition and built-in electric field.

The structure employed in this study was fabricated by MBE at TRW and is similar to profiles used for both low noise (K. L. Tan *et al*, 1990) and power applications (D. C. Streit *et al*, 1991) at 94 GHz. Grown on top of an undoped (001) GaAs substrate were 500 Å NID GaAs, 1000 Å $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$, five periods of GaAs (50 Å)/ $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ (100 Å) MQW, 3000 Å NID GaAs buffer, 150 Å $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}$ 2DEG channel, 30 Å NID $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ spacer, a sheet planar Si doping ($5 \times 10^{12} \text{ cm}^{-2}$) layer, 500 Å NID $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$, and finally 50 Å NID GaAs cap layer. Sheet electron densities of $N_s = 2.3 \times 10^{12} \text{ cm}^{-2}$ at 77 K and $N_s = 2.5 \times 10^{12} \text{ cm}^{-2}$ at 300 K were determined from Hall measurements assuming unity Hall coefficient. For the ER measurements the sample had a semitransparent (~ 50 Å) Au electrode on top of the GaAs cap and a thick Au electrode on the back surface.

Shown in Fig. 40 are the ER and PR spectra at 304 K. Three distinctive portions are well resolved in the energy domain. The features labeled A, B, and C below 1.4 eV are from the InGaAs MDQW. The structure between 1.40 and 1.45 eV is from the GaAs portion of the sample. The peaks at about 1.50 eV and 1.65 eV are from the AlGaAs cap layer (and possibly some contribution from the spin-orbit split peak of GaAs). We shall focus our attention on the InGaAs portion of the spectrum, which was related to the 2DEG channel. Note that in the PR spectrum the high energy side of peak A is more pronounced in relation to the ER trace.

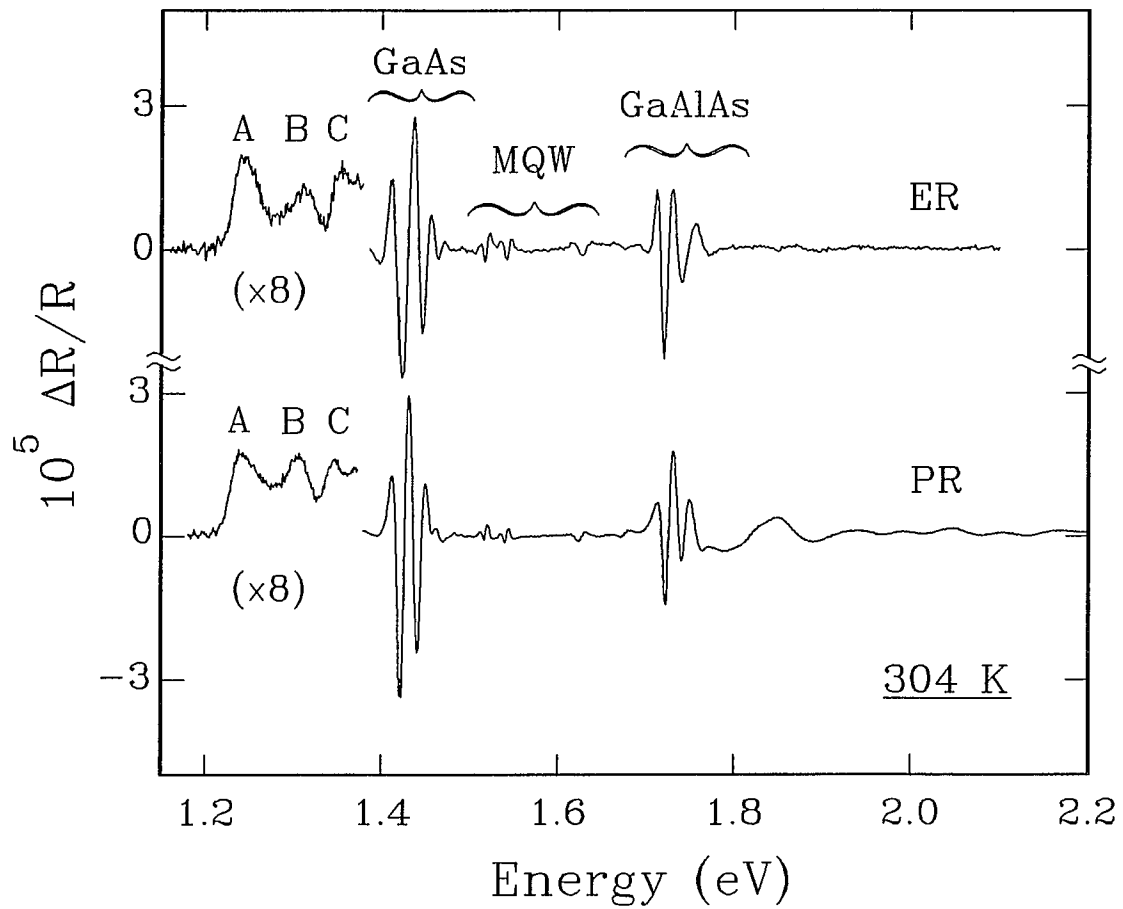


FIG. 40 ER and PR spectra from a $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}/\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ pseudomorphic HEMT structure at 304 K.

Displayed by the solid lines in Fig. 41 are the A, B, and C features of the InGaAs PR spectrum at 304 K and the ER traces at 304, 238, 148, and 79 K. The line shapes are unusual for modulation spectroscopy from a quantum well system. Such spectra generally exhibit sharp, derivative like features (i.e, positive and negative lobes) associated with excitons, even at 300 K (see for example F. Pollak, 1991 and references therein). In addition, these line shapes are symmetric (see Chapter 3). The traces of Fig. 41 lie on only one side of the baseline. Also, the peak A is asymmetric on the high

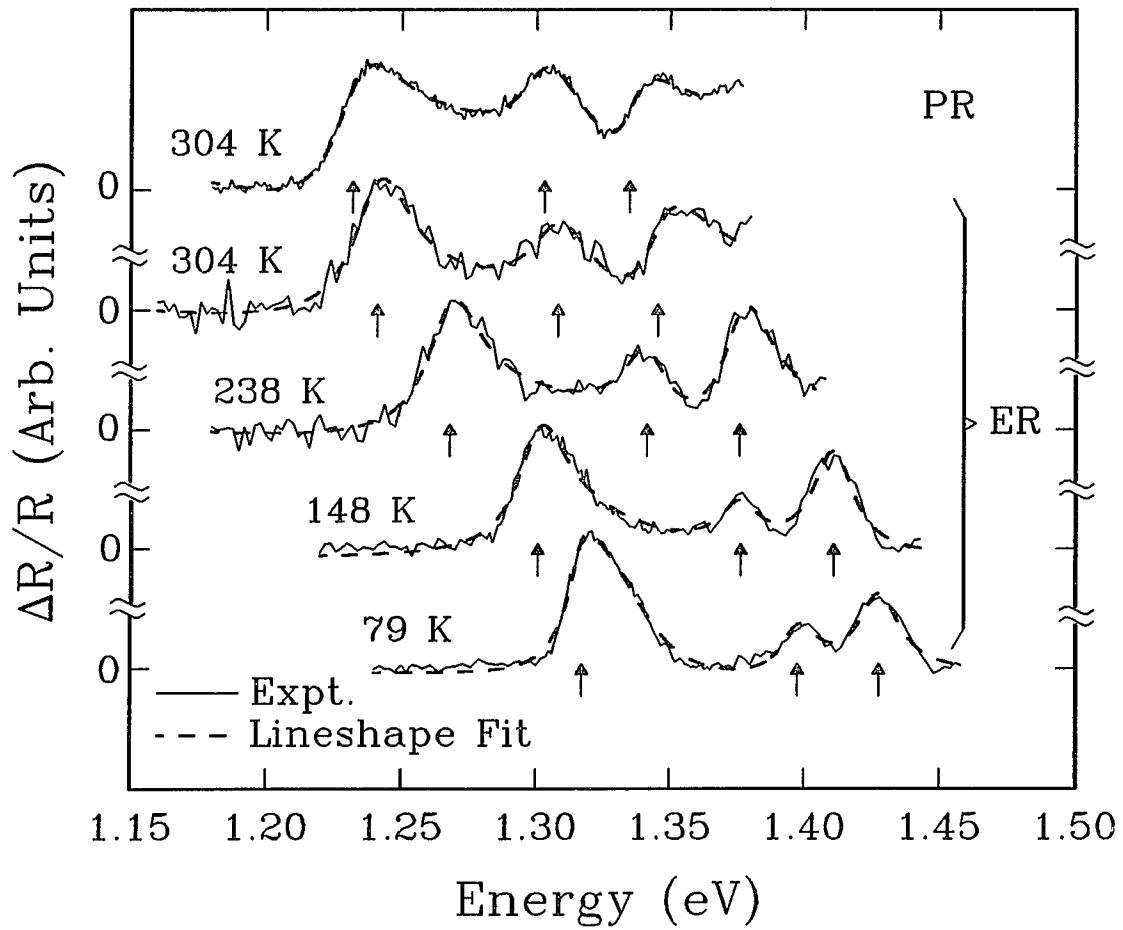


FIG. 41 Experimental PR (304 K) and ER (304, 238, 148, and 79 K) spectra below $E_0(\text{GaAs})$ from an InGaAs HEMT structure.

energy side, an effect which becomes more pronounced as the temperature is increased. As will be demonstrated below, this asymmetric property is due to the Fermi level filling factor and enables us to determine the Fermi energy.

The dashed lines in Fig. 41 are least squares fits to Eq. (3.16), which includes Fermi filling factor (see Chapter 3). The obtained intersubband energies are indicated by arrows. The asymmetry of the feature A is due to the Fermi filling factor and makes

it possible to determine $E_F - E_A^c$. We find $E_F - E_A^c = +(5 \pm 2)$, $-(6 \pm 3)$, $-(10 \pm 5)$, and $-(20 \pm 15)$ meV at 79, 148, 238, and 304 K, respectively. The error bars are larger at the higher temperatures because of the increased thermal broadening. The peaks B and C are relatively symmetric since $E_B^c - E_F$ and $E_C^c - E_F$ are larger than $k_B T$ and hence relatively insensitive to the Fermi filling factor.

Table V Various transition energies and the associated intensities (overlap integral) from a self-consistent calculation on a HEMT structure, as well as the experimental values at 79 K.

Transition	Energy (eV)		Intensity ^a (arb. unit)	
	Expt.	Calc.	Expt.	Calc.
11H ^b		1.247 (1.365 ^c)		0.11
12H ^b		1.275 (1.393 ^c)		0.24
13H ^b		1.305 (1.423 ^c)		0.32
21H	1.317 (A)	1.317	1.0	1.00
22H		1.345		0.09
23H		1.375		0.01
31H		1.377		0.21
32H	1.398 (B)	1.405	0.3	0.34
41H		1.406		0.06
42H	1.428 (C)	1.434	0.5	0.43

a. Intensities are normalized to 11H transition.

b. Not allowed at Γ point due to the Fermi level position.

c. Transition energy occurring at $k=k_F \neq 0$.

In order to identify the origins of the A, B, and C features, we have performed a self consistent theoretical calculation, including electric field effects, of the inter-

subband energies and intensities (wavefunction overlap) at 79 K (T. Ando *et al*, 1982). We assumed midgap Fermi level pinning for the free surface and GaAs buffer/MQW interface (H. Shen *et al*, 1990), a planar doping density of $5 \times 10^{12} \text{ cm}^{-2}$, an In composition of 21%, $L_z = 150 \text{ \AA}$ and a background doping level of $1 \times 10^{14} \text{ cm}^{-3}$. Exchange terms were neglected because of the carrier concentrations involved ($N_s \approx 2.5 \times 10^{12} \text{ cm}^{-2}$) (T. Ando *et al*, 1982). Details of this calculation can be found in Chapter 4 of this thesis. Listed in Table V are the theoretical results as well as the experimental values. It can be seen that there is very good agreement between experiment and theory for both energies and intensities, if we identify the spectral features A, B, and C with transitions 21H, 32H, and 42H, respectively. Transitions which involve the first electron subband are not allowed since E_F lies far above this level. We will show later that the weak signature of these transitions may still be found under suitable conditions. The overall agreement is quite good.

Based on this calculation we can determine the position of E_F relative to the electron ground state of the system. We find a value of $E_2^c - E_1^c = 70 \text{ meV}$. Since $E_F - E_2^c = +(5 \pm 2) \text{ meV}$ at 79 K and $-(20 \pm 15) \text{ meV}$ at 304 K we conclude that $E_F - E_1^c = (75 \pm 2) \text{ meV}$ and $(50 \pm 15) \text{ meV}$ at these two temperatures.

It can be shown that for the case of broadened 2D density of electron states N_s is given by:

$$N_s = \left(\frac{m_e^*}{\pi \hbar^2} \right) \sum_j \int_0^\infty dE f_e(E) \text{Im} \left[\ln(E - E_j^c + i\Gamma_j^c) \right] \quad (6.4)$$

$$f_e(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

From the data above and preceeding equation we find that $N_s = (2.2 \pm 0.2) \times 10^{12} \text{ cm}^{-2}$ at 79K and $(1.9 \pm 0.5) \times 10^{12} \text{ cm}^{-2}$ at 304 K, in good agreement with the Hall values. The decrease in E_F as the temperature is increased is consistent with the temperature dependence of the Femi energy in a 2D system (T. Ando *et al*, 1982).

We now turn our attention to the PR data at 304 K in Fig. 41. From the line shape fit of the feature A (21H) we find that $E_F - E_A^c = -(6 \pm 3) \text{ meV}$. Thus, the Fermi energy, and hence N_s , is larger than that of the corresponding ER measurement $[-(20 \pm 15) \text{ meV}]$. This is evident from the enhanced high energy tail in the PR trace compared to the ER peak. This effect is due to the presence of photoexcited carriers created by the pump beam (D. S. Chemla *et al*, 1988; G. Liveseu *et al*, 1988). Note also that the energy positions of the A, B, and C features in the PR data are red shifted by about 10 meV from the corresponding ER peaks. This is consistent with the large N_s which increases the electric field in the MDQW. The differences in the high energy component of the A structure (and also peak positions) between the PR and ER spectra can be reduced significantly by decreasing the pump light intensity by means of neutral density filters.

We have also done a detailed PR study at 300K of three step-doped $\text{Ga}_{1-y}\text{Al}_y\text{As}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ PHEMTs with nominal $y=0.2$, $x=0.2$ (samples #1 and #2) or $x=0.16$ (sample #3) and $L_z=100$ Å (Y. Yin *et al*, 1993). The structures employed in this study were fabricated by molecular beam epitaxy on undoped (001) GaAs substrates. On top of this was grown a buffer layer consisting of 4000 Å of not-intentionally doped (NID) GaAs, 300 Å of NID GaAlAs, 500 Å of NID GaAs, 100 Å of NID InGaAs which formed the MDQW, 20 Å of NID GaAlAs spacer, 200 Å and 125 Å of GaAlAs doped with Si at levels of $4.5 \times 10^{18} \text{ cm}^{-3}$ and $2 \times 10^{17} \text{ cm}^{-3}$, respectively, and a 100 Å GaAs cap with $6 \times 10^{18} \text{ cm}^{-3}$ Si doping. From the growth conditions nominal values of $y=0.2$, $x=0.2$ (samples #1 and #2) or 0.16(sample #3) and $L_z = 100$ Å were deduced. Sheet electron densities at 77K and 300K were determined for the three samples from Hall measurements assuming unity Hall coefficient. There was some variation in N_s among the three materials, as will be discussed below. The PR measurements were made at room temperature. The pump beam was the 6328 Å line of a HeNe laser chopped at 200 Hz. The pump beam power density on the sample was $1000 \mu\text{W}/\text{cm}^2$.

Shown in Fig. 42 by the solid lines are the PR spectra at 300K of samples #1,#2 and #3. The features below 1.4 eV are from the InGaAs MDQW. Also indicated are the optical signals arising from the GaAs and AlGaAs portions of the samples. We shall first focus our attention on the InGaAs region of the spectra and return to the other traces later.

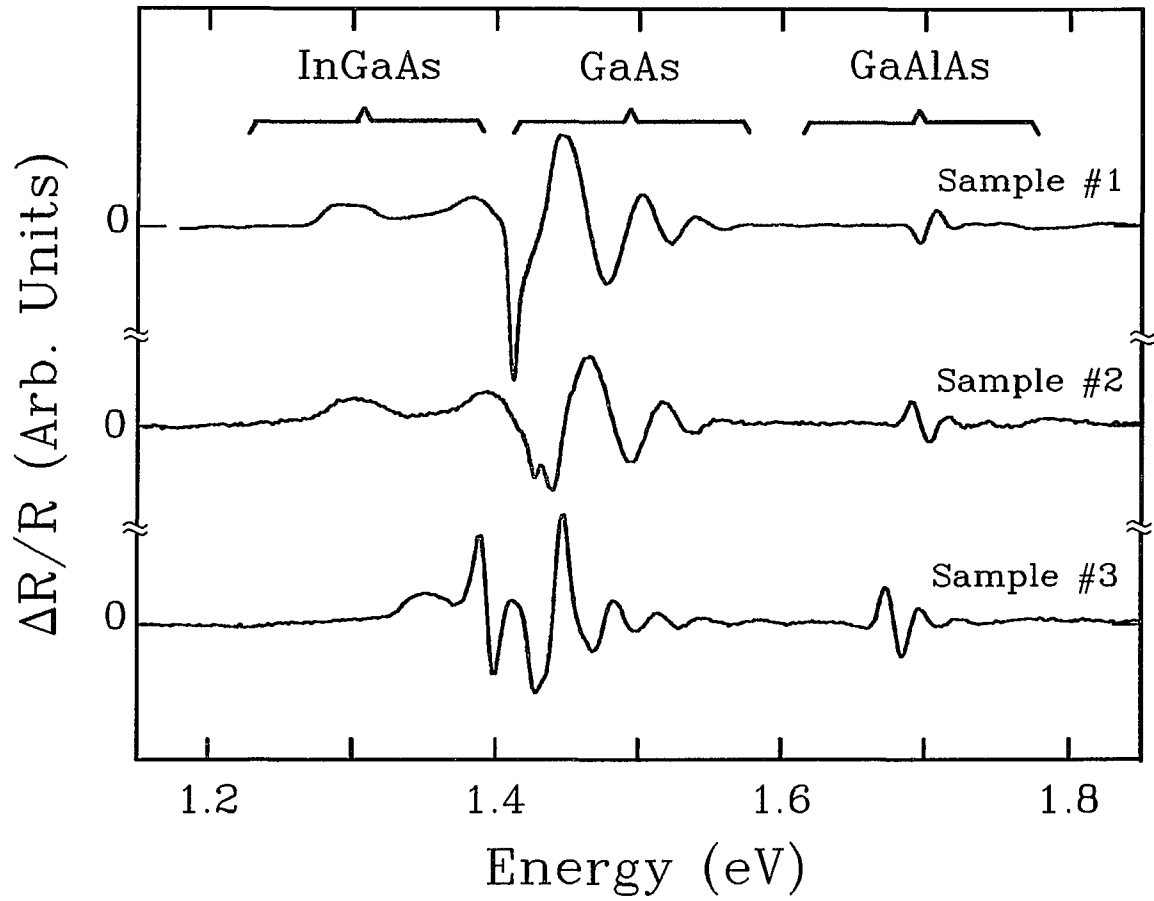


FIG. 42 Room temperature PR spectra of InGaAs HEMT structure samples #1, #2 and #3.

Displayed by the solid lines in Fig. 43 are PR spectra originating in the InGaAs MDQW section of the samples. The lineshapes are unusual for modulation spectroscopy from a quantum well (QW) system. We have similar lineshapes as in Fig. 41. The feature A in Fig. 41 shifts to higher energy as feature C in Fig. 43 since the well width is reduced from 150Å to 100Å. Also to be noted is the emergence of feature A in Fig. 43.

The dashed lines in Fig. 43 are least-squares fits to Eq.(3.16). The obtained intersubband transition energies, E_{ej} for $j = A, B, C$ and D (except for sample #3 with $j = A', B'$ and C') are indicated by arrows and also are listed in Table VI. The sharp, high energy "S" shaped structure of sample #3 (labelled D') has been fit with FDL function (dotted line). The obtained intersubband energy also is indicated by an arrow and is presented in Table VI.

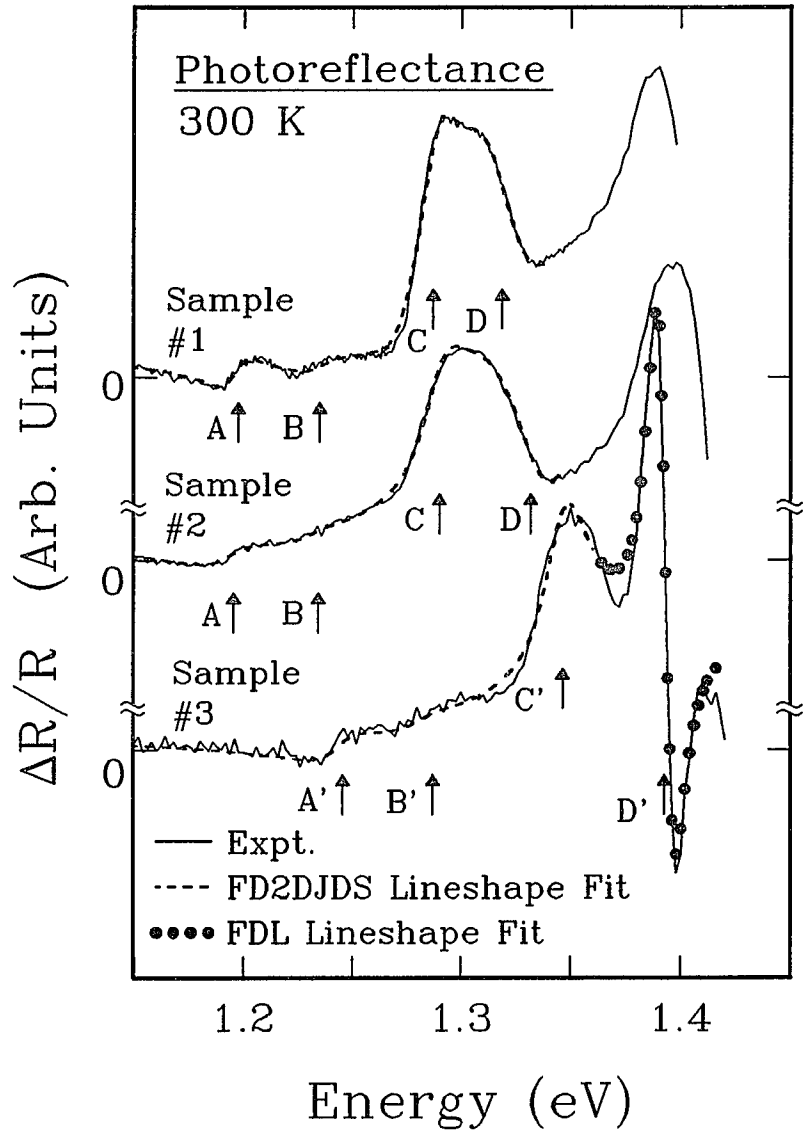


FIG. 43 Solid lines are the experimental PR spectra from the InGaAs MDQW region of the samples. The dashed and dotted lines are least squares fits to appropriate lineshape functions (see text).

As we shall demonstrate below these features for samples #1 and #2 correspond to $mnH = 11H$ ($j=A$), $12H$ ($j=B$), $21H$ ($j=C$) and $22H$ ($j=D$). The situation for sample

#3 is more complex. The background on which these resonances are superimposed is due to the Fermi filling factor, $(1-f_c^j)$. The fit to this background makes it possible to evaluate $E_F - E_A^c = 62$ meV, 71 meV and 56 meV for samples #1, #2 and #3, respectively.

In order to identify the origins (i.e., m and n) of the InGaAs MDQW features we have performed a theoretical self-consistent Schrodinger-Poisson calculation of the subband and intersubband energies and intersubband intensities (wave-function overlap)

Table VI Experimental and theoretical values of various intersubband transition energies from the InGaAs MDQW region of three $\text{Al}_y\text{Ga}_{1-y}\text{As}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ HEMTs.

Sample	Intersubband Characteristics				$N_s(10^{12} \text{ cm}^{-2})$	
	Spectral Feature	Expt. (eV)	Theory (eV)	Transition	PR Expt.	Hall Measurement
1	A	1.198	1.203 ^a	11H ^a	1.90 ± 0.20^a	1.90 ± 0.1^c 1.60 ± 0.1^f
	B	1.235	1.238 ^a	12H ^a		
	C	1.287	1.307 ^a	21H ^a		
	D	1.319	1.341 ^a	22H ^a		
2	A	1.196	1.204 ^b	11H ^b	2.15 ± 0.25^b	2.00 ± 0.1^c 1.77 ± 0.1^f
	B	1.234	1.239 ^b	12H ^b		
	C	1.292	1.307 ^b	21H ^b		
	D	1.332	1.342 ^b	22H ^b		
3	A'	1.246	1.246 ^c	11H ^c	1.85 ± 0.20^c	1.75 ± 0.1^c 1.68 ± 0.1^f
	B'	1.287	-----	(12H) ^{c,d}		
	C'	1.346	1.341 ^c	21H ^c		
	D'	1.393	-----	(22H) ^{c,d}		

a. $y=0.195$, $x=0.2$.

b. $y=0.185$, $x=0.2$.

c. $y=0.175$, $x=0.16$.

d. The 2H valence level is unbound.

e. 77K.

f. 300K.

including the influence of the large electric field in the InGaAs MDQW (see Appendix A). This calculation was based initially on the doping profiles of growth condition, $L_z = 100\text{\AA}$ and a background doping level of $1 \times 10^{14} \text{ cm}^{-3}$ for the NID region. The other parameters, i.e., x and y , are indicated in Table VI. The In composition was taken to be the intended growth value while the Al content was deduced from the energy position of the AlGaAs peak (see Fig.42). The $\text{In}_x\text{Ga}_{1-x}\text{As}$ band gap and InGaAs/GaAs band offset were taken from S. H. Pan *et al* (1988), the out-plane masses from W. Zhan *et al* (1991), the deformation potentials were a linear interpolation between those of GaAs and InAs (F. H. Pollak, 1990).

These theoretical results are listed in Table VI. For samples #1 and #2 the overall agreement is very good if we identify feature A with 11H, etc. For sample #3 the feature A' and C' can be correlated with 11H and 21H, respectively. We shall return to the question of the nature of B' and D' below.

Also based on this calculation we can determine the position of E_F relative to the electron ground state ($m=1$) of the system. Since $m=1$ for the feature A, we can determine that $E_F - E_A^c = E_F - E_1^c$. Hence, from the above mentioned fitted results we conclude that $E_F - E_1^c = +62 \text{ meV}$, $+71 \text{ meV}$ and $+56 \text{ meV}$ for samples #1, #2 and #3, respectively. The quantity $E_2^c - E_1^c (\approx 100 \text{ meV})$ can be obtained from the separation between 21H and 11H (see Table VI). Thus the Fermi level lies between the $m=1$ and $m=2$ conduction subbands.

From Eq. (6.4) and the values of E_F and E_m^c discussed above we have calculated the numbers for N_s for the three samples listed in Table VI. Values for Γ_m were taken from the lineshape fits in Fig. 43. There is very good agreement between the PR analysis of N_s and the 77K Hall measurements, which also are displayed in Table VI. For completeness we also list in Table VI the N_s values from the 300K Hall determinations.

We now return to the question of sample #3. Because of the lower In content of this sample in relation to the other two materials the 2H valence level becomes unbound and hence m2H transitions should be very weak in a one electron picture. However, experimentally we still see in Fig. 43 evidence for the contribution of 12H (feature B') and a very strong resonance (D') which appears to correspond to 22H. The fact that the D' structure has a lineshape of FDLL strongly suggests that its origin is an unscreened exciton. Clearly further work needs to be done with regard to this peak.

Both the GaAs and AlGaAs features in the PR spectra of Fig. 42 exhibit pronounced FKOs. The electric fields (in units of 10^4 V/cm) deduced from the GaAs FKOs are 4.7, 5.3 and 3.1 while from the AlGaAs FKOs we find 1.6, 1.8 and 1.8 for samples #1, #2 and #3, respectively.

Also from the position of the AlGaAs peaks of 1.695 eV, 1.689 eV and 1.672 eV (see Fig. 42) we can evaluate the Al compositions (T.F. Kuech *et al.*, 1987) to be

19%, 18.5% and 17.5% for samples #1, #2, and #3, respectively. These values are in reasonably good agreement with the intended numbers.

From the self-consistent Schrodinger-Poisson calculation we also can determine the built-in electric fields in the GaAs and AlGaAs portions of the sample. Based on midgap Fermi level pinning at the 500Å NID GaAs/300Å NID AlGaAs interface we determine a field of about 7.6×10^4 V/cm in the 500Å GaAs region. This is somewhat larger than the fields deduced from the FKOs. This observation suggests that the pinning level is less than midgap and is about 0.30-0.35 eV below the conduction band.

The FKOs associated with the AlGaAs signal originate in the 300Å NID AlGaAs portion next to the 4000 Å NID GaAs buffer. If we assume that the Fermi level at the 300 Å NID AlGaAs/ 4000 Å NID GaAs buffer interface is not pinned near midgap but is about 0.30-0.35 eV above the valence band, a uniform field of approximately 2×10^4 V/cm will be present in this region of the sample. This number is close to our experimental values. The AlGaAs layers above the InGaAs channel are all fairly heavily doped and the field in this space charge region is about 2×10^5 V/cm, about an order of magnitude larger than our experimental values. The FKOs from this region are probably not observable because of the high doping levels (H. Shen and F. Pollak, 1990).

In conclusion we have performed a detailed ER and PR study of the AlGaAs/InGaAs/GaAs HEMT structures. The features associated with the InGaAs MDQW exhibit unusual traces which can be accounted for on the basis of a two dimensional density of states (screened excitons) and a Fermi level filling factor. From a detailed line shape fit, particularly to the high energy side of the lowest lying feature at 79 K, we have been able to deduce the Fermi energy and hence N_s . The latter is in good agreement with a Hall effect measurement. The general trends of E_F with temperature and light intensity are consistent with the properties of a 2DEG. Comparison of the obtained intersubband energies with a theoretical calculation also makes it possible to deduce other important parameters such as L_z , In composition and built-in electric field. The energy resolved signals from the GaAs and AlGaAs regions reveal more information about the structures.

From the GaAs and AlGaAs optical structures we have been able to deduce corresponding electric fields and Al composition. The field related to the GaAs signal is in reasonable agreement with a calculation of the built-in fields. The PR determination of the Al composition also confirms the intended growth conditions.

Low temperature PL also has been used to characterize pseudomorphic modulation-doped structures. S. K. Brierly *et al* (1991) reports a correspondence between the linewidth of the 22H feature at 77K and the electron sheet density. Gilperez *et al* (1992) have correlated the observed PL (10K) energy shifts of the 11H and 21H

transitions and intensity of the 11H feature with N_s . Zhang and Ploog (1992) as well as Dodabalapur *et al* (1989) have found a relation between the linewidth of the single observed PL peak (6K) and the electron sheet density.

Our work demonstrates the considerable utility of EM in characterizing these pseudomorphic HEMT structures. The ability to perform measurements at room temperature in a contactless, non-destructive manner (PR) has considerable implications for process control. For example, wafer sized samples can now be conveniently evaluated before being processed into actual devices. In addition, the low light levels used in PR in relation to PL will reduce any spurious effects on the evaluation of N_s due to photo-excited carriers.

Furthermore, the fact that measurements can be performed over a very broad temperature range, means that many fundamental 2DEG phenomena, such as the Fermi edge singularity (S. Schmitt-Rink *et al*, 1989; G. Livescu *et al*, 1988; W. Chen *et al*, 1992) and temperature dependence of E_F (T. Ando *et al*, 1982), can be explored.

6.4 Summary

Electric field is an essential primary effect in most real devices. The thorough understanding of various effects can usually be benefited in short term. Several understanding of electric field related phenomena in semiconductor microstructures from this work are summarized here:

- In SQW structure, a electric field plays its role in two areas.
 - (a) A near quadratic red shift of fundamental transition energy (QCSE).
 - (b) The relative changes of intensities of various transitions. The original allowed transitions disappear while the "forbidden" transitions gain strength due to the breakdown of parity conservation by the presence of electric field.

- In a symmetrical CDQW structure, an electric field can tune the inter-well resonance coupling besides its role of QCSE inside each well. We observed the following phenomena from our experiments:
 - (a) Resonance coupling between energy levels of two wells at flat band condition $F=0$.
 - (b) With the application of electric field, this resonance coupling is destroyed. All the inter-well like transitions undergo huge Stark shifts and lose their intensities, while the reverse is true for the intra-well like transitions. Because of the intensity change, a blue shift of the absorption edge is obtained.
 - (c) The coupling resonance between different sub-levels, e.g., 2H-3H, is possible if the appropriate field is reached.
 - (d) Under excessively large field, two sets of the surviving intra-well transitions are degenerate and undergo normal QCSE while the intensities are further weakening. The linewidth is significantly broader due to field

induced tunneling.

- (e) The line shape analysis has shown to be a valuable aid in identifying the nature of various features. The gap modulation mechanism is found to be dominant across the low field as well as medium field regions. The positive or negative field dependence of transition energies divide all the features into two categories. Each category has its positive or negative lobe distinction revealed on the spectra. The 12H feature, which changes its field dependence during the course of the field change, reveals this change on the experimental spectra as it changes its category belonging.
- The work on the HEMT structure has to deal with the free electron carriers of 2DEG besides the built-in electric field. Modulation spectroscopy has shown itself to be a valuable tool of the study in this area.
 - (a) The 2DEG related features of AlGaAs/InGaAs/GaAs HEMT are well isolated in the energy domain from the rest of features.
 - (b) An unusual line shape is found to be associated with the 2DEG features. The developed line shape is a first derivative 2D screened exciton modified by Fermi distribution function, which agrees well with the experimental data.
 - (c) A self-consistent Schrodinger-Poisson numerical solver is developed. The calculated results can be used to aid the understanding of experimental data.

- (d) Relative Fermi level position is possible to be extracted from the observed asymmetrical 2DEG feature of the experimental data. Based on this knowledge together with the theoretical understanding of electron sub-level separations, 2DEG carrier density N_s can be evaluated. This approach has been justified by comparing with the Hall measurement results.
- (e) Optical features from GaAs and AlGaAs layers can give more valuable information about the structure.

Chapter 7. Uniaxial Stress Effect -Static Properties

7.1 Introduction

The application of uniaxial stress to a semiconductor produces changes of the lattice parameter and symmetry properties of the material. The uniaxial stress effect on a bulk semiconductor has been well established with the successful deformation potential theory. For example, in a diamond or zinc blende type material, the stress Hamiltonian for the Γ_1 conduction band can be expressed as:

$$H_\epsilon^c = a_c(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \quad (7.1)$$

where a_c is the deformation potential and ϵ_{ij} ($i, j=1,2,3$) is the strain component. The stress Hamiltonian for the Γ_{15} valence band can be written down as (F. H. Pollak, 1990):

$$H_\epsilon^v = -a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) - b[(L_z^2 - \frac{1}{3}L^2)\epsilon_{zz} + c.p.] - \sqrt{3}d[(L_xL_y + L_yL_x)\epsilon_{xy} + c.p.] \quad (7.2)$$

where a_v , b , and d are the deformation potentials corresponding to the hydrostatic (O_h), tetragonal (D_{4h}), and trigonal (S_6 , C_{3i}) deformations, respectively, L_i ($i=1,2,3$) is the angular momentum operator of i th component, and $c.p.$ is the cyclic permutation.

The effect of a [001] or [111] stress on the E_0 transition, for instance, will generate a hydrostatic pressure effect and lift the valence band degeneracy of HH and LH bands at Γ point by shear components (deformation potentials b or d).

In spite of its proven utility, little work has been done on the effects of uniaxial stress (**S**) on the properties of heterostructures. Several authors have performed stress measurements on (001) GaAs/AlGaAs MQWs up to 5 kbar (see Fred H. Pollak, 1990 and references therein). Until recently, no work has been done on strained layer systems. We have carried out extensive research works in this area on various material systems. In section 7.2, I will briefly describe the uniaxial stress set up. I will describe our works on AlGaAs/GaAs epilayer, InGaAs/GaAs SQW, GaAs/AlGaAs SQW, and GaAs/Si in section 7.3.

In the beginning of this project, we examined the GaAs substrate wafers and an $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}/\text{GaAs}$ epilayer structure. The outcome was encouraging. We were able to achieve comparable stress magnitude on the thin wafered samples as thick bulk samples. The work on thin film microstructures is thus possible. And since modern growth techniques produce better quality samples, measurements of improved accuracy are possible. The recently results on these testing bulk materials (wafers) will be presented in section 7.3.1.

Uniaxial stress on microstructures is an attractive topic. We have applied in-plane stress on an InGaAs/GaAs SQW in both [100] and [110] directions. The quantum confinement and built-in biaxial strain due to the lattice mismatch defined the preferred z axis along the growth direction, while the external applied uniaxial stress tries to pick up its own z axis. The competition between them results in an interesting situation for

various studies including fundamental studies of quantum theory. We achieved up to 18 kbars on a strained InGaAs/GaAs SQW. This superior stress magnitude as compared to the other reported ones (usually around 5 kbar, see for example F. H. Pollak, 1990 and references therein) enabled us to (a) unambiguously identify LH transitions from both the shifting speed and polarization selection behavior at high stress and (b) observe the phenomena associated with the QCSE generated by piezoelectric effects in the [110] case. These activities will be covered in section 7.3.2.

In view of the piezoelectric effect in InGaAs/GaAs SQW structure as well as the large achievable stress magnitude, we revisited the GaAs/AlGaAs QW structures in section 7.3.3. SQWs were chosen instead of MQW to eliminate extra uncertainties. We observed some phenomena which has not been previously reported on this system such as the stress dependent polarization behavior on intensity and partial screened piezoelectric effect.

GaAs material system grown on Si substrate is a promising attempt on combining the advantages of optical and electrical performance of these two materials. In view of its built-in biaxial tensile stress, this system forms a counterpart of InGaAs/GaAs system. In studying this material, we do find a pronounced anticrossing behavior. Because of its strong resonance coupling as compared to the SQW subbands (e.g., 11L-13H), an interesting polarization behavior (optical anisotropy) is also observed. These results will be discussed in section 7.3.4.

We will use $E_0(1)$ (LH along stress axis) and $E_0(2)$ (HH along stress axis) notations for Bulk origin signals while using the $mnH(L)$ notations for features originating from the QWs in order to avoid confusion. Generally, $E_0(2)$ and mnL features have larger stress dependence. The different stress dependence makes the uniaxial stress a powerful tool of determining the HH or LH characters of optical transitions. The (001) z axis will always be chosen along the growth direction.

Growth directional stress is desirable due to its higher symmetry property. Since the stress direction and built-in strain/confinement are collinear, the HH and LH bands are still well defined in this situation. In another word, the j and m_j remain good quantum numbers. We have worked out a modification to our stress apparatus to include this configuration. Some preliminary experimental results are encouraging and they will be briefly discussed in section 7.3.5.

7.2 Experimental Setup

It is a home made setup with its history way back to the 60s. The exceptionally excellent design enables us to achieve routinely up to 10-20 kbars on GaAs material systems. The schematic diagram is shown in Fig. 44.

The sample slice under test is carefully mounted and restricted between a fixed and a sliding pistons inside a sample frame. The external force is manually adjusted by a spring device on the right, which is magnified by the level arm on the top. This force

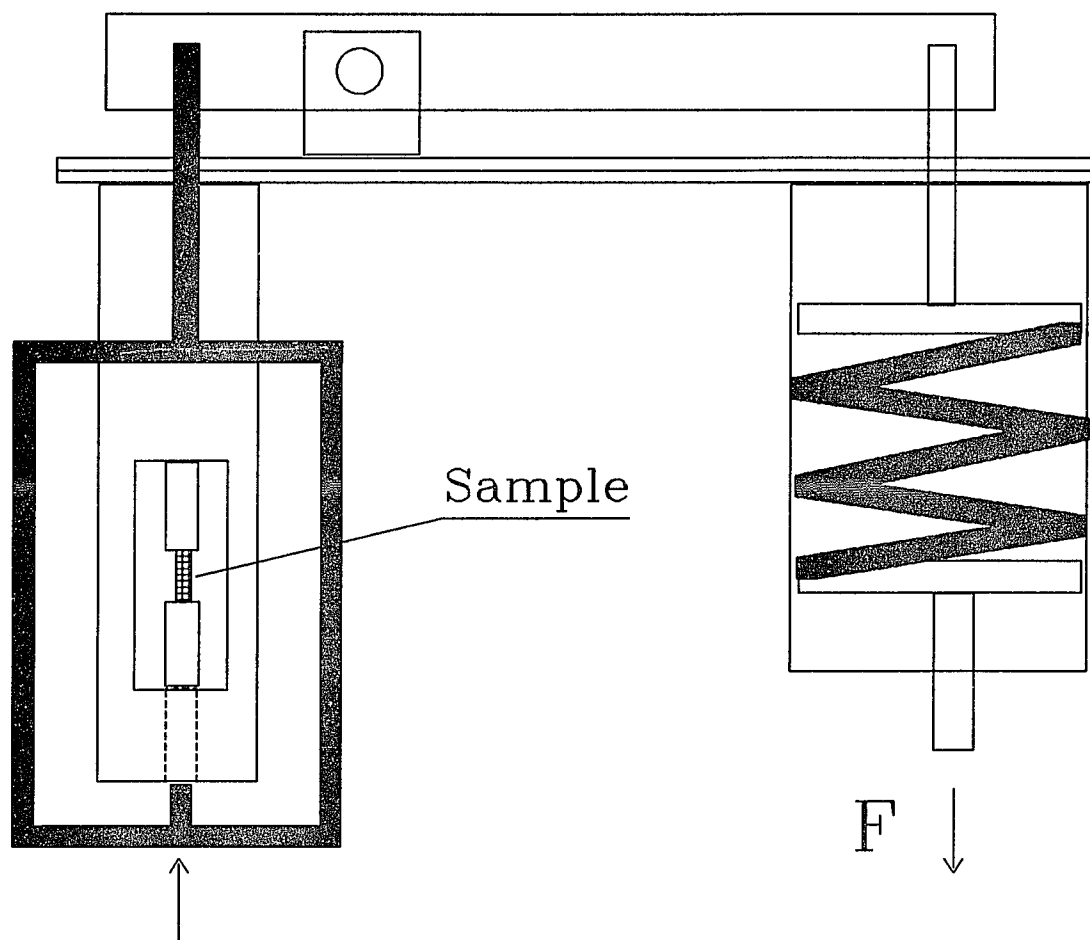


FIG. 44 Schematic diagram of the uniaxial stress setup.

is then transferred through a rigid pulling frame onto a pin point that is located at the bottom of the fixed sample frame. This pin pushes the sliding piston upward to squeeze the sample, resulting in a uniaxial stress distribution on the center portion of the sample. A sensitive bridge circuit monitors the elongation of the primary spring and thus the amount of force generated. The whole system has been carefully calibrated and the reproducibility is excellent. The experimental error on the stress magnitude (<0.05 kbar) is mainly limited by the error on the sample cross sectional area, owing to the facts of both the thin thickness wafer sample deployed and the fluctuation from imperfect

sample contour.

The samples studied so far are all [001] grown structures. For uniaxial stress study, the samples are typically 2mm wide and 15mm long and oriented along either [100] or [110] by X-ray backscattering to better than 1° . The details of the sample preparation is described in section 2.4.

7.3 Experimental Results

7.3.1 Deformation Potential Measurements on GaAs and AlGaAs/GaAs Epilayers

We have investigated the effects of compressive uniaxial stress on the PR spectra of the fundamental direct band gap (E_0) and its spin-orbit component ($E_0 + \Delta_0$) of GaAs and $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ (H. Qiang *et al*, 1990). The transitions were studied at 300 K for S parallel to [100] and [110], including polarization effects. From the stress induced shifts and splittings, we have been able to deduce the hydrostatic (a) and shear (b and d) deformation potentials of these materials. Although GaAs has been studied extensively, this is the first investigation of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ under large, variable external stress.

The semi-insulating GaAs samples were cut from a [001] commercial wafer of thickness 0.5mm fabricated by the liquid encapsulated Czochralski method. Such material is frequently employed as a substrate for the fabrication of various thin film GaAs based structures. No special treatment was given to the surface. The AlGaAs sample is an epitaxy on a [001] GaAs buffer and substrate.

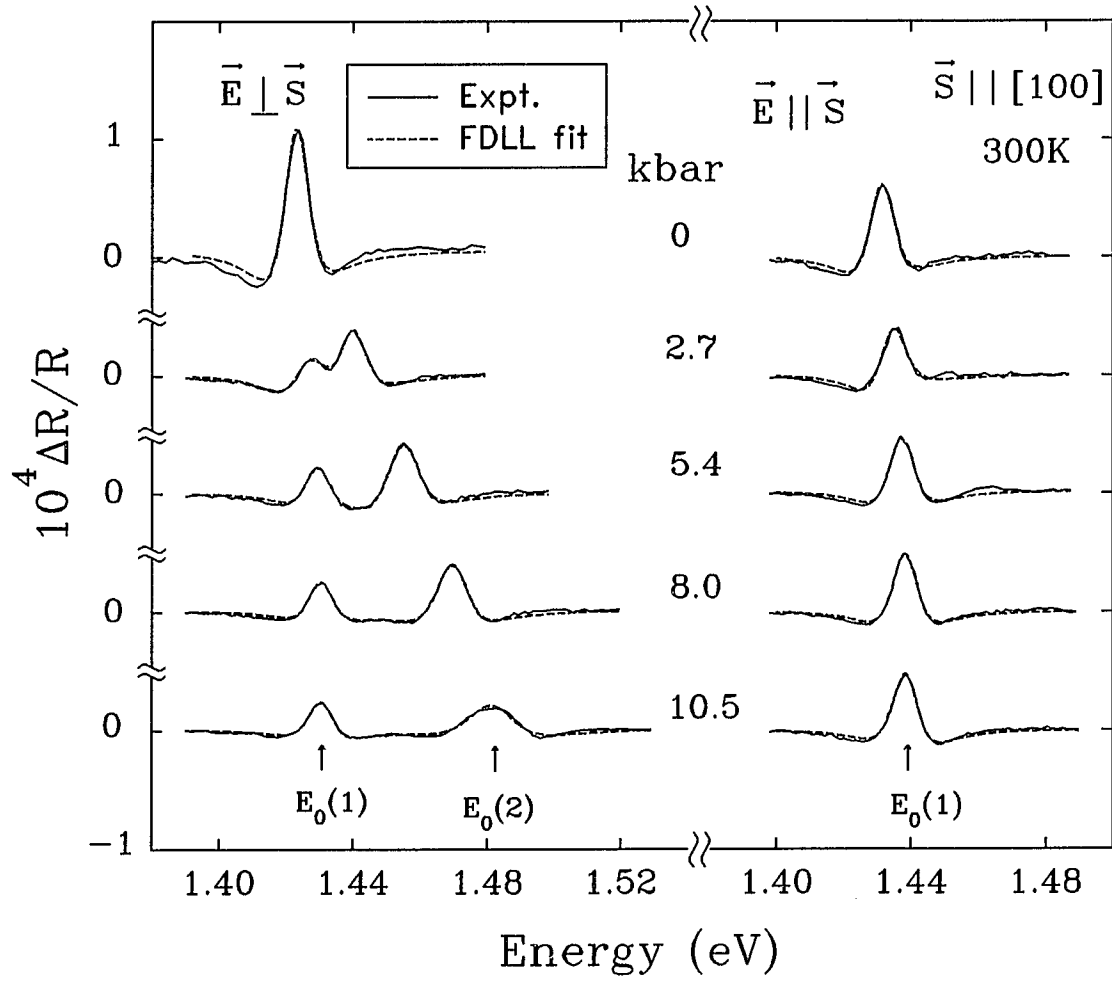


FIG. 45 PR spectra (solid lines) of GaAs at various stresses for both $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$ with $\vec{S} \parallel [110]$ at 300K. Dashed lines are fits to the FDLL.

PR spectra of GaAs under uniaxial stress were taken for both $\vec{S} \parallel [100]$ and $\vec{S} \parallel [110]$ at 300 K. Shown in Fig. 45 are the PR spectra of $\vec{S} \parallel [110]$ for both (a) $\vec{E} \perp \vec{S}$ and (b) $\vec{E} \parallel \vec{S}$. The original single feature at $S=0$ is split into a doublet of $E_0(1)$ and $E_0(2)$. The $E_0(1)$ feature is relatively insensitive to the stress and can be observed in both polarizations, while the $E_0(2)$ feature has strong dependence on the stress and can be only observed for $\vec{E} \perp \vec{S}$. At large stress, the intensity ratio agrees with the magic numbers 1:3:4:0 (see Table VII).

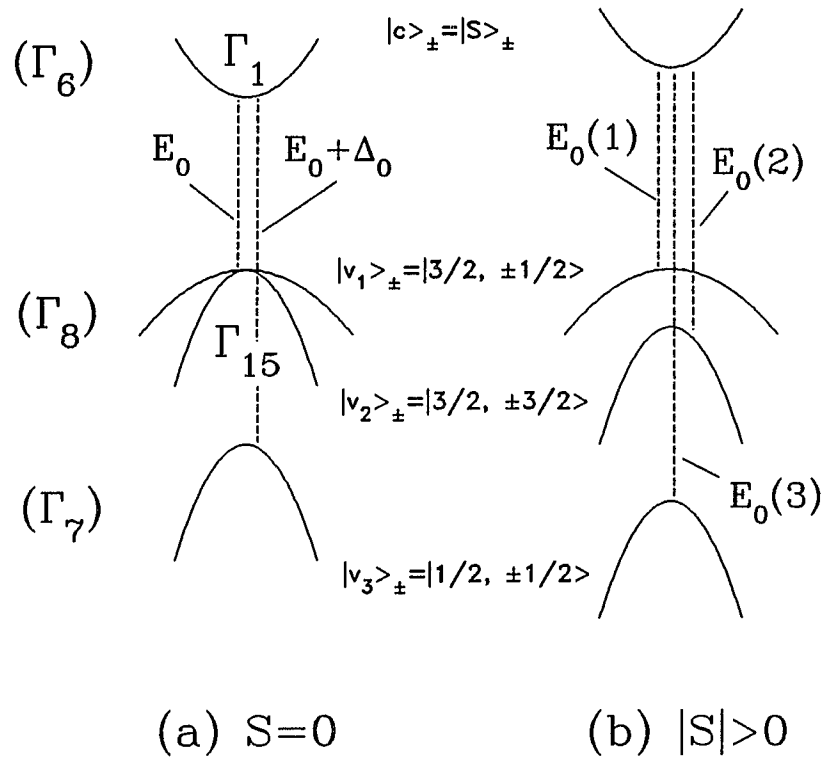


FIG. 46 Schematic band diagram around E_0 of a zinc-blende type material for both (a) without S and (b) with $S \parallel [100]$.

In order to understand the experimental observations, the band structure is shown for GaAs near E_0 region in Fig. 46 for (a) without S and (b) $S > 0$ for $S \parallel [100]$. For a free standing ($S=0$) Zinc-blende type material like GaAs, the conduction band is a Γ_1 singlet while the Γ_{15} valence bands consist of a degenerate doublet and a spin-orbit-split singlet with the two fold Kramers degeneracy. Because of the degeneracy of $|3/2, \pm 1/2\rangle$ and $|3/2, \pm 3/2\rangle$ at Γ point, the valence bands have warped energy surfaces. For example, shown in Fig. 47(a) are the calculated in-plane valence band dispersions for bulk GaAs near Γ point at $S=0$.

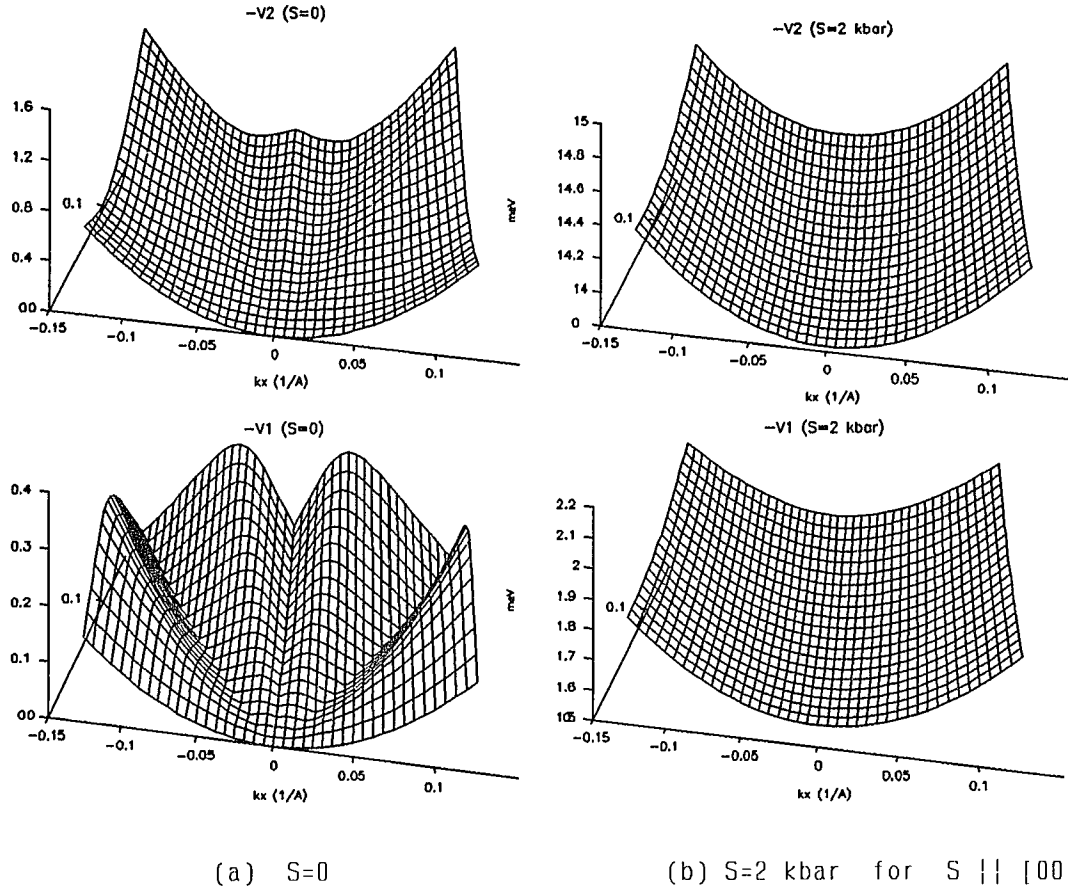


FIG. 47 Calculated bulk GaAs valence band dispersions at $k_z=0$ near Γ point for (a) $S=0$ and (b) under external uniaxial stress $S \parallel [100]$ with $S=2$ kbar.

A uniaxial stress, as shown on the right of Fig.

46, splits the $J=3/2$ multiplet into a pair of degenerate Kramers doublets. The three separate valence bands are labeled v_1 , v_2 ,

and v_3 . The transition between the conduction band and the valence band v_i is denoted $E_0(i)$, where $i=1,2,3$. The stress dependence of the relative intensities of these

Table VII Intensities of $E_0(1)$, $E_0(2)$, and $E_0(3)$ transitions of Zinc-blende type materials under external uniaxial stress.

	$E \perp S$	$E \parallel S$
$E_0(1)$	$1(1-4\gamma)$	$4(1+2\gamma)$
$E_0(2)$	3	0
$E_0(3)$	$2(1+2\gamma)$	$2(1-4\gamma)$

a. In unit of $P^2/6$.

b. $\gamma = \delta E_{100}/\Delta_0$ for $S \parallel [100]$ and $\gamma = \delta E_{111}/\Delta_0$ for $S \parallel [111]$.

transitions are listed in Table VII for $\mathbf{E} \parallel \mathbf{S}$ and $\mathbf{E} \perp \mathbf{S}$, which can be deduced from the wavefunction symmetry properties (F. H. Pollak, 1990). The removal of the $J=3/2$ degeneracy produces ellipsoidal energy surfaces with the symmetry axis along the uniaxial stress direction. The calculated valence band structures of GaAs under $S = 2\text{kbar}$ are plotted in Fig. 47(b).

Shown in Fig. 48(a) are the stress dependent energies of $E_0(1)$ and $E_0(2)$ for GaAs for $\mathbf{S} \parallel [100]$ obtained from the least squares fits to PR spectra of both $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$. $E_0(3)$ energies are also displayed. However, since $E_0(3)$ is weaker than the former two transitions no polarization dependent studies were made for this feature. Representative error bars are shown. The solid lines are least squares fits to Eqs. (4.19). Based on the linear stress dependence coefficients and using $C_{11} = 1.19 \times 10^{12}$ and $C_{12} = 5.38 \times 10^{11}$ of J. S. Blakemore (1982), we have determined the deformation potentials a and b . These results are listed in Table VIII. In Fig. 48(b) is displayed similar data for $\mathbf{S} \parallel [110]$. The solid lines are least squares fits to Eqs. (4.20) which produce a and d since b is known from the $[100]$ data. The non-linear terms for $E_0(2)$ are very small and hence we did not detect any quadratic dependence on S . These results are also listed in Table VIII.

Similar experiments were done on an $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}/\text{GaAs}$ epilayer structure. Since this is a lattice matched system and the difference of elastic moduli between the two materials is negligible, the deformation pattern of $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ layer under uniaxial

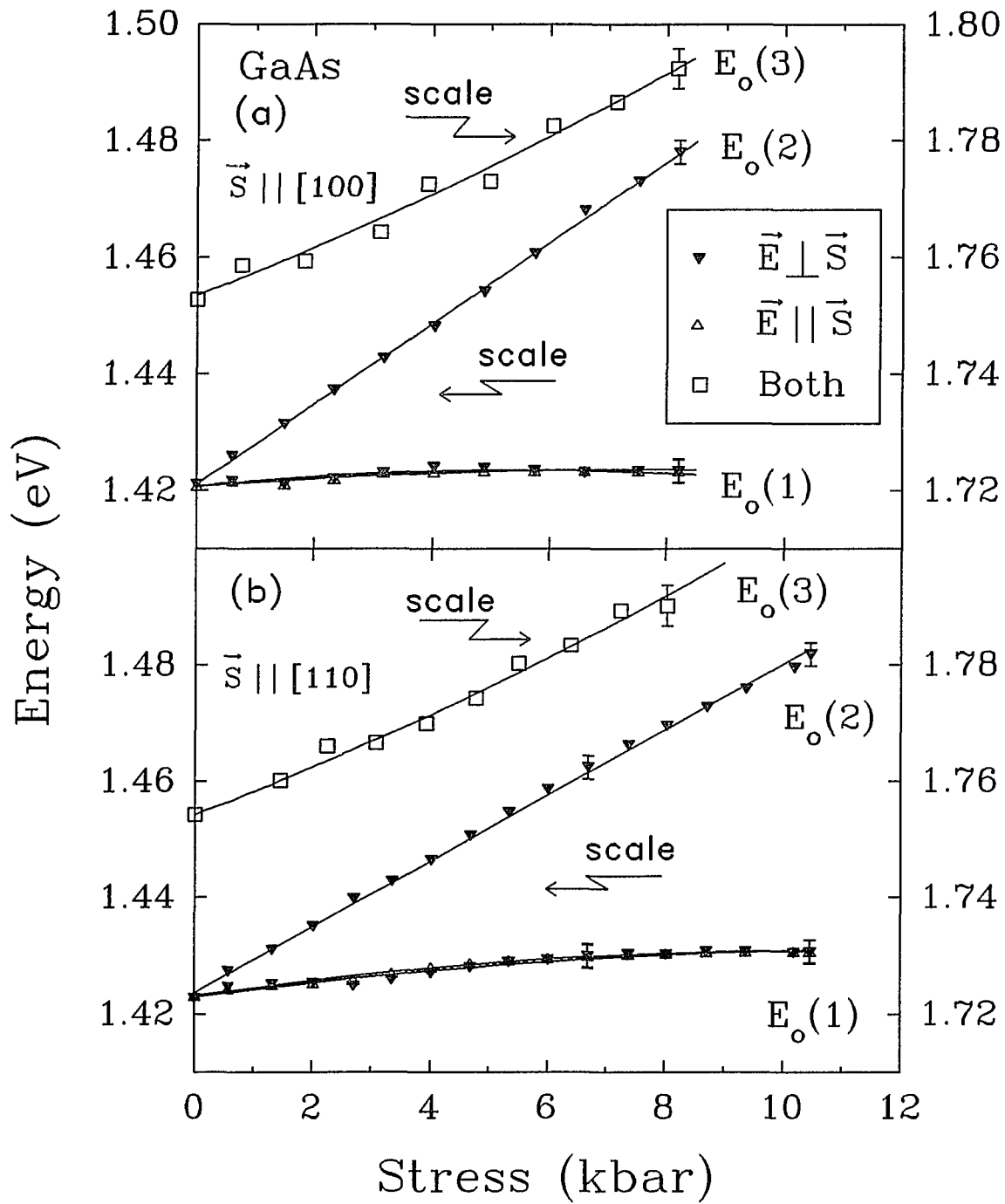


FIG. 48 Stress dependent $E_0(1)$, $E_0(2)$, and $E_0(3)$ of GaAs for (a) $\vec{S} \parallel [100]$ and (b) $\vec{S} \parallel [110]$ at 300K.

Table VIII Deformation potentials for the E_0 transition in GaAs.

	This Work	Previous Work	Theoretical Calculations
a (eV)	8.72 ± 0.2^a 8.81 ± 0.2^d	6.36^b 6.70^b 8.46^b 9.43^b	7.2^c 8.8^c 12.0^e 13.5^f
b (eV)	2.00 ± 0.2^a	1.7^b 2.9^b	2.2^f 1.6^g
d (eV)	4.43 ± 0.6^h	4.55^b 5.4^b 5.3^b	4.2^f 5.3^g

- a. $S \parallel [100]$; using $C_{11} = 1.19 \times 10^{12}$ dyn/cm² and $C_{12} = 5.38 \times 10^{11}$ dyn/cm² of Blakemore (1982).
- b. F. H. Pollak (1990).
- c. M. Cardona and N. Christensen (1987).
- d. $S \parallel [110]$; using $C_{11} = 1.19 \times 10^{12}$ dyn/cm² and $C_{12} = 5.38 \times 10^{11}$ dyn/cm² of Blakemore (1982).
- e. B. Vinter (1986).
- f. A. Blacha *et al* (1984).
- g. P. Pfeffer *et al* (1984).
- h. Deduced from the $S \parallel [110]$ results with b from the $S \parallel [100]$ data; using $C_{44} = 5.95 \times 10^{11}$ dyn/cm² of Blakemore (1982).

stress is essentially identical to a pure $Al_{0.22}Ga_{0.78}As$ bulk material, which is unavailable to us. Thus, by using a standard treatment of that used on GaAs, the properties of bulk $Al_{0.22}Ga_{0.78}As$ can be studied on this epilayer.

Shown in the Fig. 49 and Fig. 50 are the PR spectra of $Al_{0.22}Ga_{0.78}As$ taken at 300 K for $S \parallel [100]$ and $S \parallel [110]$, respectively. Data was taken with the probe beam polarized both perpendicular ($\perp$) and parallel ($\parallel$) to the stress axis. The stress induced shift, split, and polarization behavior are all well presented in the experiment spectra. The

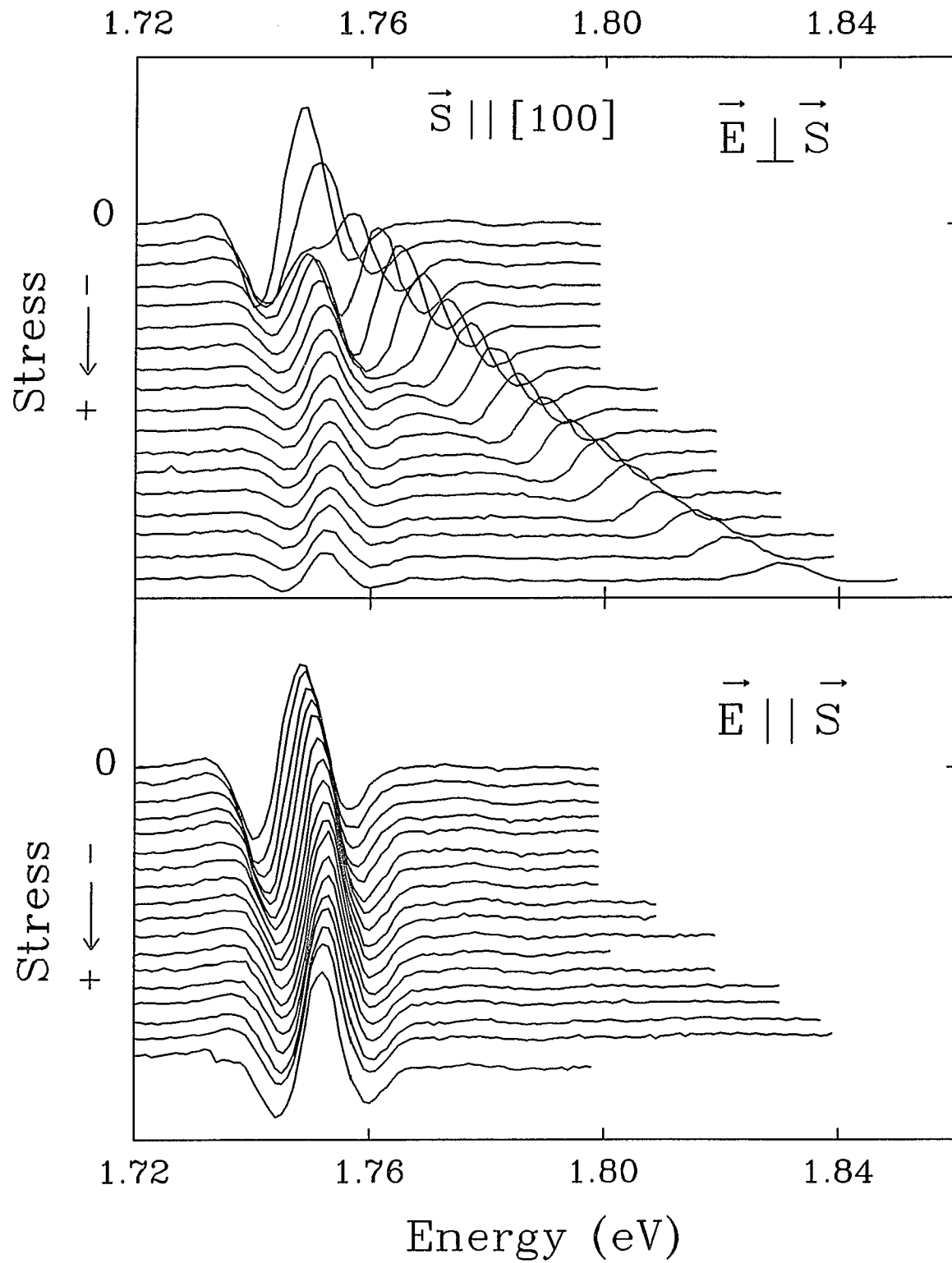


FIG. 49 PR spectra of $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ at various stresses for both $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$ with $\vec{S} \parallel [100]$ at 300K.

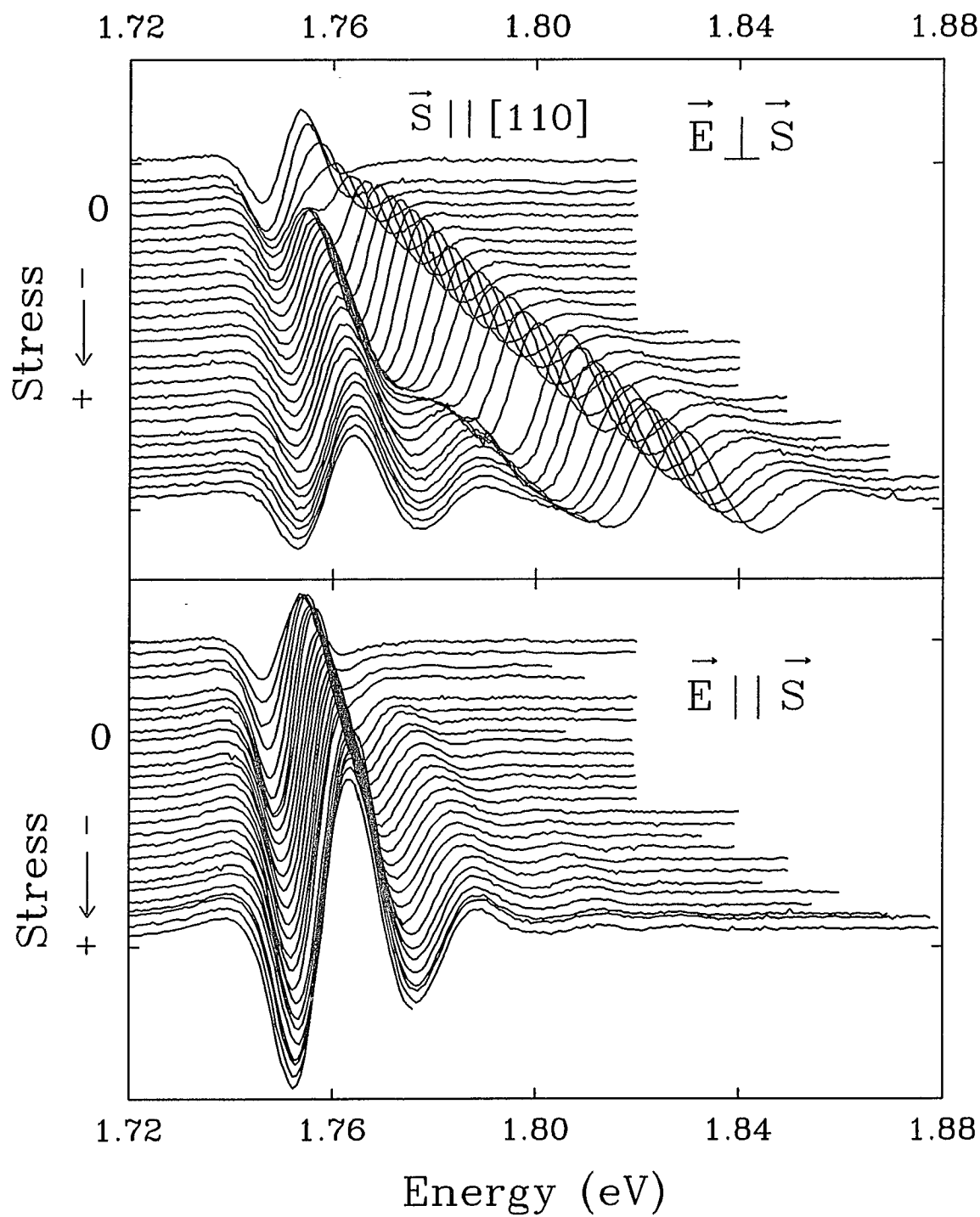


FIG. 50 PR spectra of $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ at various stresses for both $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$ with $\vec{S} \parallel [110]$ at 300K.

difference of the line shapes between the $S \parallel [100]$ and $S \parallel [110]$ spectra, notably the development of high energy wings for $E \parallel S$ of $S \parallel [110]$, is due to the partial screened piezoelectric effect (FKO).

Table IX Deformation potentials for the E_0 transition in $Al_{0.22}Ga_{0.78}As$.

	This Work	Previous Work	Theoretical Calculations
a (eV)	10.85 ± 0.2^a 10.60 ± 0.2^d	9.11 ± 0.2^b	7.24^c
b (eV)	2.08 ± 0.2^a	1.88^e 1.86^f 2.1^g	
d (eV)	5.47 ± 0.6^h		

- a. $S \parallel [100]$.
- b. Evaluated from $a = (1/3)(C_{11} + 2C_{12})(dE_0/dP)$ where (dE_0/dP) for $Al_{0.22}Ga_{0.78}As$ was taken from N. Lipshitz *et al* (1979).
- c. Linear interpolation of $a(GaAs) = 7.2$ and $a(AlAs) = 7.4$ from M. Cardona and N. Christensen (1987).
- d. $S \parallel [110]$.
- e. S. Logothetidis *et al* (1989) with $b(Al_xGa_{1-x}As) = 1.76 + 0.5x$.
- f. S. Logothetidis *et al* (1989) with $b(Al_xGa_{1-x}As) = 1.7 + 0.6x$.
- g. S. Logothetidis *et al* (1989) with $b(Al_xGa_{1-x}As) = 2.0 + 0.5x$.
- h. Deduced from the $S \parallel [110]$ results with b from the $S \parallel [100]$ data.

Plotted in Figs. 51(a) and 51(b) are the results for $Al_{0.22}Ga_{0.78}As$ for $S \parallel [100]$ and $S \parallel [110]$, respectively. Representative error bars are shown. For this material $E_0(3)$ was very weak and hence no reliable results could be obtained. The solid lines in these figures are again the least squares fits, yielding a , b , and d for this material. These values are listed in Table IX.

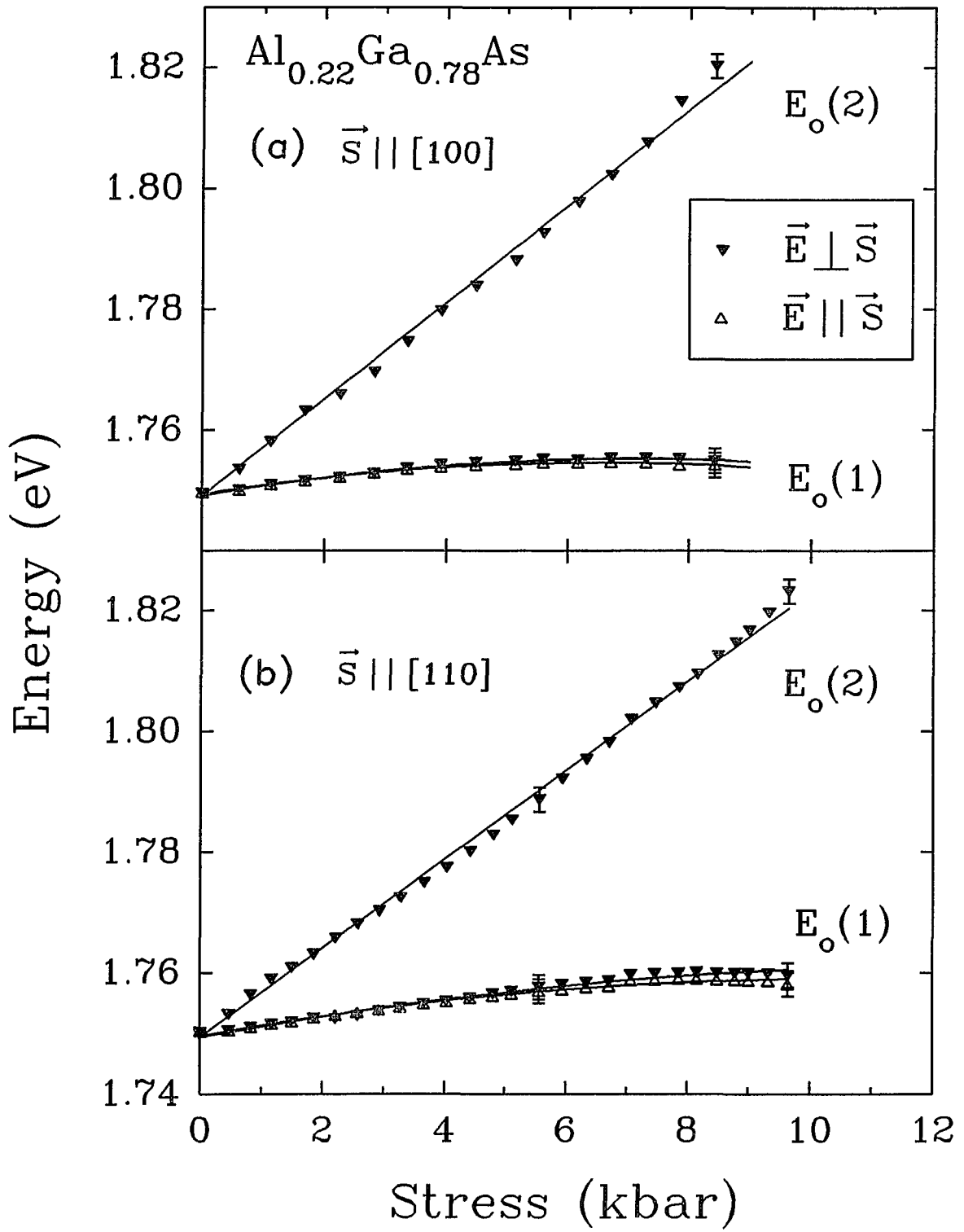


FIG. 51 Stress dependent $E_0(1)$ and $E_0(2)$ of $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ for (a) $\vec{S} \parallel [100]$ and (b) $\vec{S} \parallel [110]$ at 300K.

In addition to the values of a , b , and d for GaAs and $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ obtained in this experiment we have also listed in Table VIII and Table IX previous experimental as well as theoretical determinations.

Our numbers for GaAs are in good agreement with prior evaluations. In particular, our result for b is probably more accurate than previous investigations since a detailed line shape fit was used in our work to obtain the energies of the various transitions. In previous stress dependent modulation experiments (I. Balslev, 1972; F. H. Pollak, 1973, 1990) only peak positions were employed for data analysis. Also because of the better sample quality (narrower Γ) available now, $E_0(1)$ and $E_0(2)$ are well resolved (no overlap) even at small S (see Fig. 45). The quantity d has large error bars since it was deduced from the $[110]$ measurement which involves a linear combination of b and d rather than from a $S \parallel [111]$ experiment which depends only on d .

To date little work has been done concerning the effects of strain on the direct band gap E_0 of $\text{Al}_x\text{Ga}_{1-x}\text{As}$. Lipshitz *et al* (1979) have reported the shift of absorption edge of AlGaAs with hydrostatic pressure. Our value of a is somewhat larger than their value as well as the theoretical predictions of M. Cardona and N. Christensen (1987). Logothetides *et al* (1989) determined b for this alloy system from a study of the splitting of the direct gap exciton due to the lattice mismatch in $[001]$ AlGaAs/GaAs grown by LPE. These authors find that $b(\text{Al}_x\text{Ga}_{1-x}\text{As}) = b(\text{GaAs}) - 0.5x$. Using $b(\text{GaAs}) = 2.00$ we

obtain, using their relationship, $b(\text{Al}_{0.22}\text{Ga}_{0.78}\text{As})=2.10$, in good agreement with our experimentally obtained value listed in Table IX.

Previous uniaxial stress works on thin film GaAs/AlGaAs materials reported values of only about 4 kbar (J. Lee *et al*, 1988; B. Gil *et al*, 1988). This work demonstrates that stress comparable to those of bulk samples ($\approx 10\text{kbar}$) (F. H. Pollak, 1990) can be achieved on our setup.

In conclusion, we have measured the effects of an externally applied stress along [100] and [110] on the PR spectra of the direct gaps of GaAs and $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}/\text{GaAs}$ thin film samples. From the stress induced splittings and shifts we have deduced the deformation potentials a , b , and d . For GaAs our results agree very well with previous works. For $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ our value of a is somewhat larger than that obtained from hydrostatic pressure measurements and from a theoretical calculation. For b the value deduced in this experiment agree with the Al composition dependence reported by S. Logothetidis *et al* (1989). This is the first evaluation of d in this material. Our experiment also demonstrates that stress can be applied to thin samples ($\approx 0.5\text{mm} \times 2\text{mm}$ cross section) fabricated from substrate material that are comparable to previous works on samples ($\approx 1.5\text{mm} \times 1.5\text{mm}$) cut from bulk semiconductors.

The measured deformation potentials of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ternary materials are summarized in Table X for several Al compositions. The $x=0.27$ is obtained on the

Table X Experimental deformation potentials of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ternary alloy with different Al compositions.

Al composition	a	b	d
0^a	8.7 ± 0.2 8.8 ± 0.2	2.0 ± 0.2	4.4 ± 0.6
0.22^a	10.9 ± 0.2 10.6 ± 0.2	2.1 ± 0.2	5.5 ± 0.6
0.27^b	8.6 ± 0.2	1.9 ± 0.2	

a. This work.

b. See Section 6.3.3.

AlGaAs barrier signal of a GaAs/AlGaAs SQW structure (see section 7.3.3). A discontinuity of the parameters around 0.22-0.27 is suggested from the table. Similar observation was reported by N. Lipshitz *et al* (1979). This issue needs further investigation.

7.3.2 Stress Effects on Biaxially Compressed InGaAs/GaAs SQW System

Recently there has been considerable interest in the properties of strained layer QWs and SLs, such as InGaAs/GaAs with a [111] growth axis. Such structures have large internal fields generated by the piezoelectric effect. These internal electric fields substantially change the electronic band structure and optical properties of (111) QWs and SLs and can lead to large nonlinear optic and electro-optic effects. These fields cause a tilting of the energy bands and creat a red shift of the optical transition energies (QCSE) and changes in the oscillator strength (E. A. Caridi *et al*, 1990). Goossen *et al* (1990) have reported a room temperature blue shift with an applied voltage in a (111) $\text{In}_{0.1}\text{Ga}_{0.9}\text{As}/\text{GaAs}$ *p-i-n* MQW modulator. Because of symmetry considerations such

strain generated electric fields are not allowed in (001) strained layer systems (see for example D. L. Smith and C. Maihiot, 1990).

We have found a piezoelectric effect generated in a (001) strained $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW by an external stress (S) along $[110]$ (H. Qiang *et al*, 1991, 1992b). We have measured the effects of large $S \parallel [110]$ (~ 18 kbar) as well as $S \parallel [100]$ (~ 8 kbar) on the optical properties of the SQW. Using PR at 300K, we have studied the stress induced changes in the energies and intensities of a number of intersubband transitions. For $S \parallel [110]$ we have observed a red shift of a number of peaks and a dramatic increase in the amplitudes of several "symmetry forbidden" heavy hole features. This was not seen for $S \parallel [100]$. We interpret this phenomenon as being due to an electric field along $[001]$ induced by the piezoelectric coupling for S along the lower symmetry $[110]$ direction. In contrast to the piezoelectric fields induced in (111) strained layer systems, this effect can be (a) externally tuned in a contactless manner and (b) observed in lattice matched microstructure systems such as (001) and (111) $\text{GaAs}/\text{AlGaAs}$.

The SQW sample was fabricated by MBE in a Varian Gen-II system in IBM T. J. Watson Research Center. The fabrication condition indicates an In composition of 20% and a well width of $100\text{\AA}$. The high quality of this sample is indicated by the fact that at 10K the linewidth of the fundamental 11H exciton transition is only 2 meV. This

value is close to the theoretical limit for alloy scattering and hence contains little contribution from interfacial roughness (Y. S. Huang *et al*, 1991b).

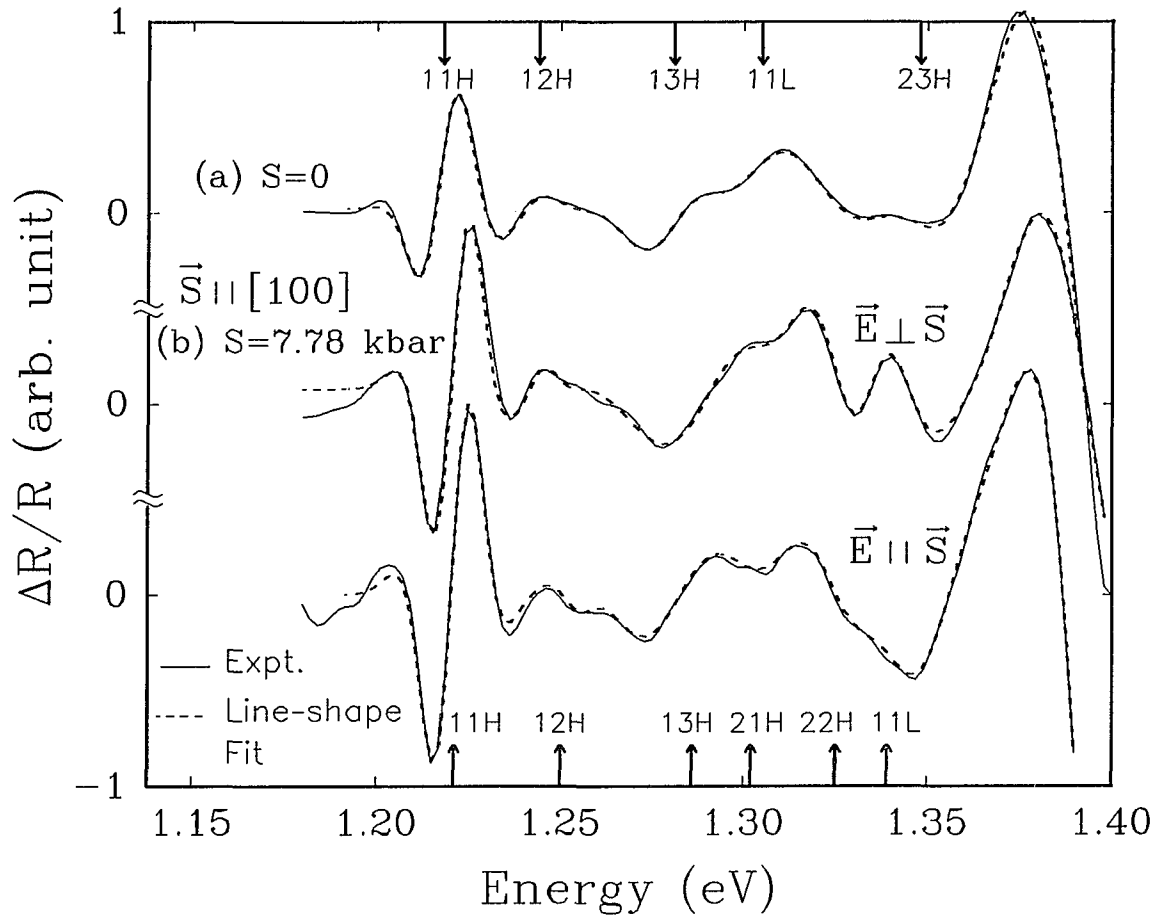


FIG. 52 PR spectra of an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW at 300K for (a) $S=0$ and (b) $S=7.8$ kbar along $[100]$ for $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$.

Shown in Fig. 52(a) is the PR spectrum (solid line) of the sample at 300K for $S=0$. The dashed line is a least squares fit to a FDGL function. The obtained energies are denoted by arrows at the top of the figure. We have identified the origin of these various features $mnH(L)$ by comparison with an envelope function calculation, including strain (G. Bastard and A. Brum, 1986). The best overall fit was obtained for an In

composition of 21 % and a well width of 105Å. These values are also in good agreement with an X-ray measurement (Y. S. Huang *et al*, 1991b). The lowest lying feature is the symmetry allowed 11H transition. At about 1.30eV there is a structure which actually contains two oscillators, i.e., 11L and 22H, both of which are symmetry allowed. The remaining features in the spectrum are due to symmetry forbidden transitions such as 12H, 13H, and 23H. Although 13H is symmetry forbidden it is parity allowed because of the finite depth of the well (Z. M. Fang *et al*, 1988). The presence of 12H and 23H is probably due to a small built-in electric field in the sample. The large feature starting at around 1.38eV corresponds to the direct gap of the GaAs cap/substrate/buffer.

The solid lines in Fig. 52(b) are the PR spectra at 300K for a stress of 7.8 kbar along [100] for light with the electric field vector $\mathbf{E}$ polarized perpendicular ($\perp$) and parallel ($\parallel$) to the external stress $\mathbf{S}$. The dashed lines are least squares fits to the FDGL function. The obtained energies are indicated at the bottom of the figure.

A comparison of Figs. 52(a) and 52(b) shows that the energies of the heavy hole transitions (11H, 12H, 13H) are relatively insensitive to the external stress while 11L has shifted to higher energies and is seen only for $\mathbf{E} \perp \mathbf{S}$. The stress dependence of the various transitions are similar to that observed for (001) GaAs/AlGaAs MQWs for $\mathbf{S} \parallel [100]$ (see for example F. H. Pollak 1990 and references therein), while the polarization dependence has not been reported on any semiconductor microstructures before.

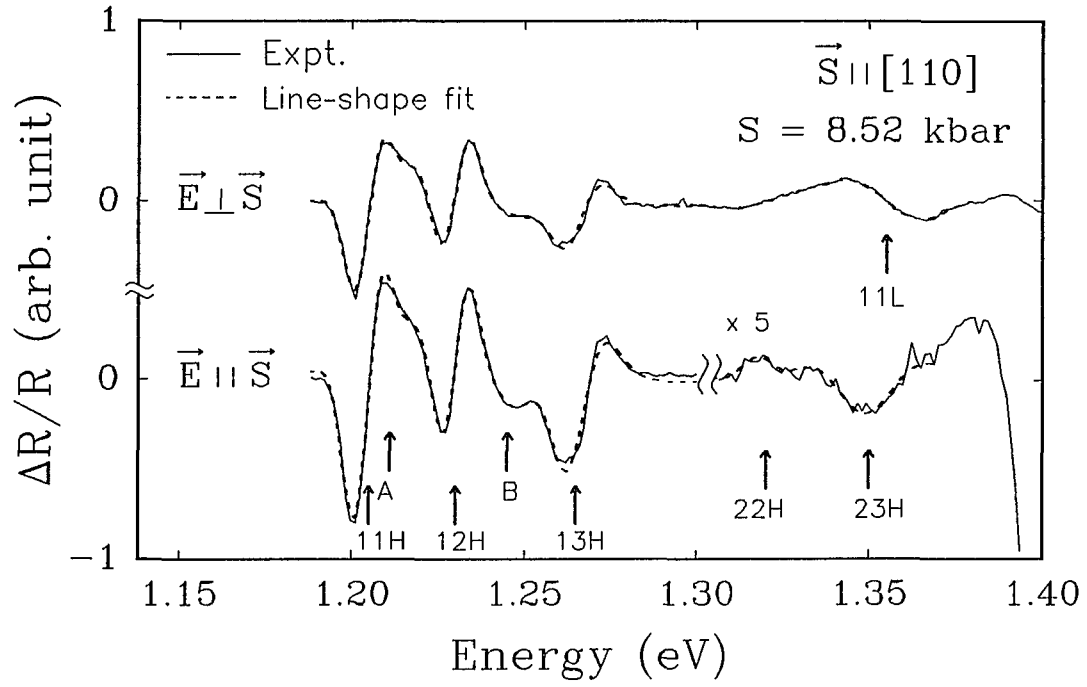


FIG. 53 PR spectra of an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW at 300K for $S=7.6$ kbar along $[110]$ for $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$.

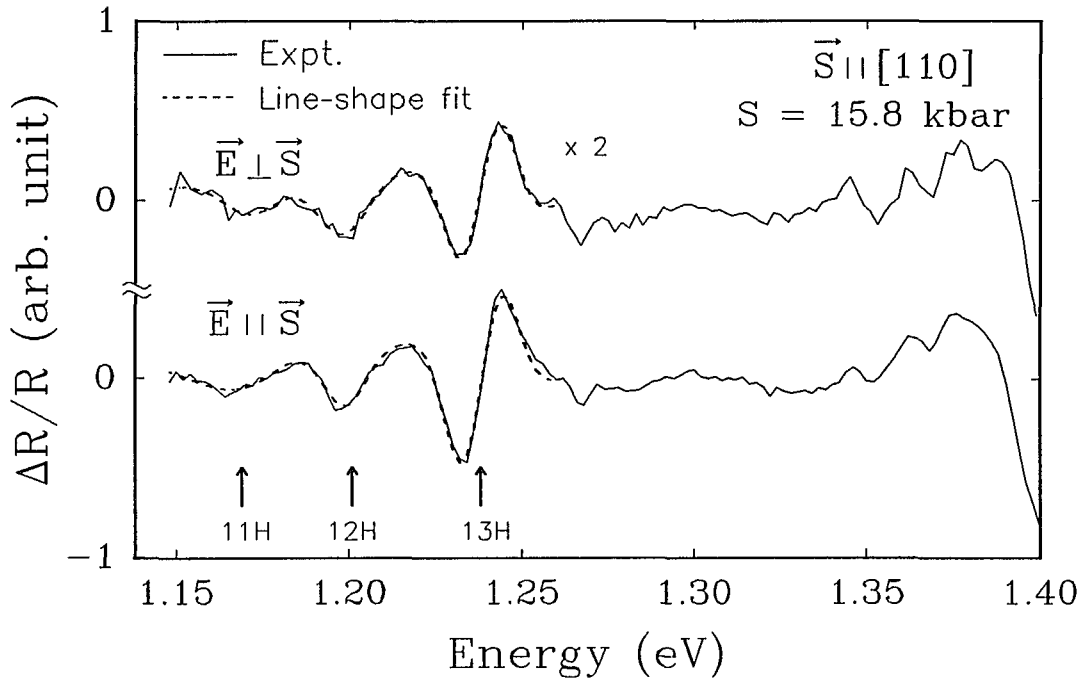


FIG. 54 PR spectra of an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW at 300K for $S=15.8$ kbar along $[110]$ for $\vec{E} \perp \vec{S}$ and $\vec{E} \parallel \vec{S}$.

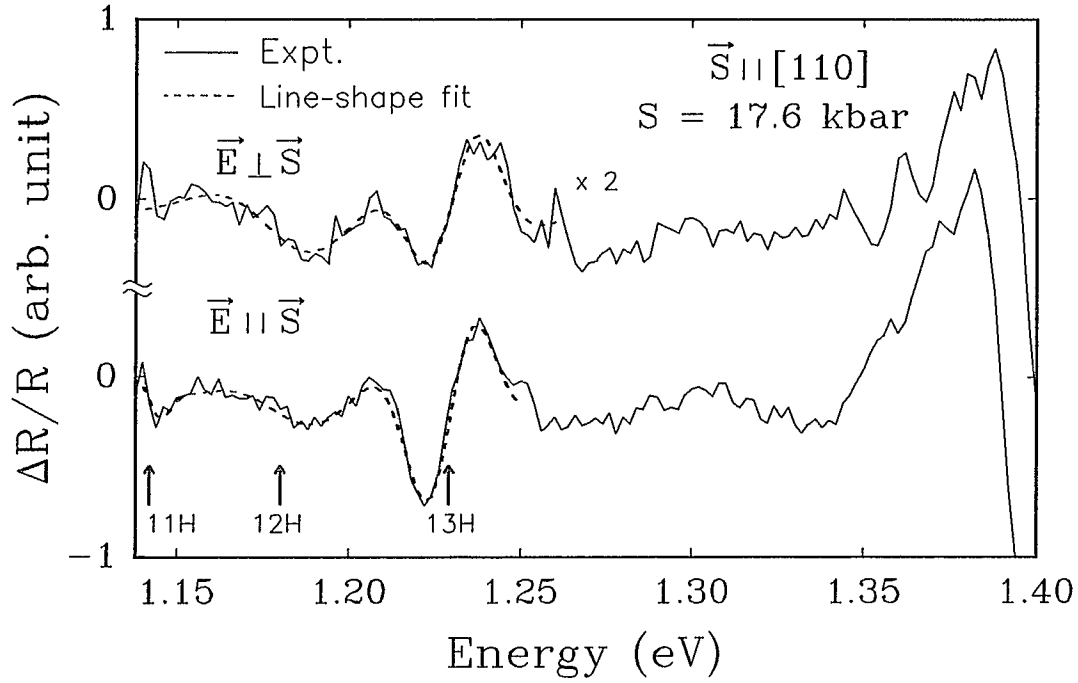


FIG. 55 PR spectra of an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW at 300K for $S=17.6$ kbar along $[110]$ for $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$.

Displayed by the solid lines in Figs. 53-55 are the experimental data for $\mathbf{S} \parallel [110]$ for 8.5, 15.8, and 17.6 kbar, respectively, for $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$. The dashed lines are least squares fits to the FDGL function. What is most significant about these spectra is the dramatic change in the amplitude of the symmetry forbidden 12H and 13H features in relation to the symmetry allowed 11H and 11L transitions. This effect is not observed for $\mathbf{S} \parallel [100]$ (see Fig. 52). For the highest stress there is also a considerable red shift of the heavy hole peaks due the quantum confined Stark effect (D. A. B. Miller *et al*, 1986) related to the piezoelectric field. Those effects have not been observed in previous piezo-optical experiments on quantum wells because of the low stresses (~ 5 kbar) that were employed (F. H. Pollak, 1990; J. Lee *et al*, 1988; B. Gil *et al*, 1988). In Fig. 53 the polarization dependence of 11L is clearly evident. Another interesting aspect of

Fig. 53 is that the lowest lying heavy hole features have split into doublets designated (11H, A) and (12H, B), respectively. A similar effect has been observed in a (001) GaAs/AlGaAs MQW structure for $\vec{S} \parallel [100]$ (J. Lee *et al*, 1988). Although the exact origin of the A and B peaks is not known they might be due to excited states (e.g., 2s) of the 11H and 12H excitons or $\vec{k} \neq 0$ transitions (J. Lee *et al*, 1988). These peaks are under further investigation.

The stress induced shifts in energy of the various features for $\vec{S} \parallel [100]$ are in good agreement with a theoretical calculation of the effects of external stress on the electronic levels of SQW implicitly including coupling with the spin-

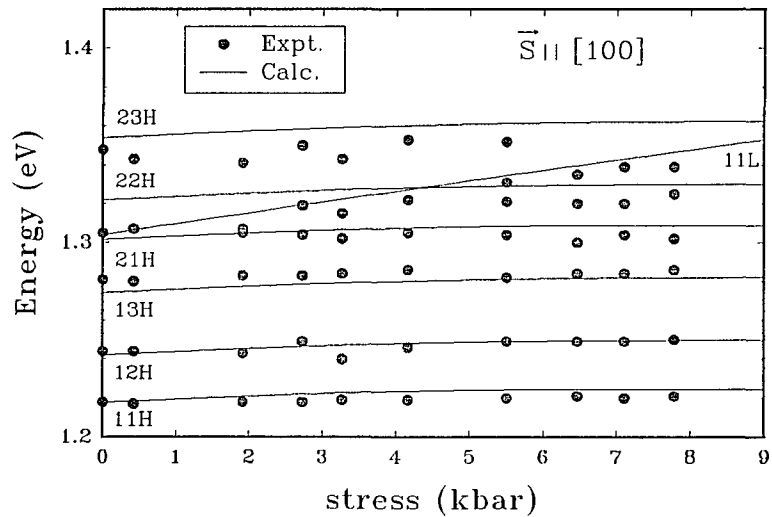


FIG. 56 Stress dependent energies of various quantum transitions in an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW for $\vec{S} \parallel [100]$.

orbit-split band. They are shown in Fig. 56. However, a similar analysis is not able to explain the result for $\vec{S} \parallel [110]$. Notice the discrepancy between the experimental values and the calculated stress dependence (dashed line) of 11H feature shown in Fig. 57. A huge red shift is observed.

We interpret the above stress induced red shifts and changes in the amplitudes of 11H, 12H, and 13H for $S \parallel [110]$ as being due to an external piezoelectric effect along the [001] growth axis. For Zinc-blende materials the off-diagonal strains produce a polarization field given by (D. L. Smith and C. Mailhot, 1990; W. F. Cady, 1946)

$$F_z = \left[\frac{e_{14}}{2\kappa\epsilon_0 C_{44}} \right] S \quad (7.3)$$

where e_{14} is the piezoelectric constant, κ is the dielectric constant, ϵ_0 is the permittivity of free space, and C_{44} is the elastic moduli. For a 17.6 kbar stress along [110], a field of 1.85×10^5 V/cm can be generated in the $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}$ layer (H. Qiang *et al*, 1991, 1992b). This field is large enough to account for the observed red shift as well as the intensity changes.

In order to confirm the above interpretation of the effects for $S \parallel [110]$ we have performed a theoretical calculation including not only the effects of strain, similar to $S \parallel [100]$, but also the influence of the stress generated F_z on the energy levels (QCSE) and intensities of 11H, 12H, and 13H. Interested readers are referred to Chapter 4 for the detailed calculation method. The relaxation method was employed to determine the QCSE and the overlap integrals (intensities) between the valence and conduction subband wave functions.

Shown in Fig. 57 by solid lines are the results of this calculation. An overall good agreement on the amount of red shifts of various transitions can be seen. The

support of this QCSE interpretation also lies on the intensity changes. Shown in Fig. 58 by the solid lines are the calculated intensities (wavefunction overlap) of 11H, 12H, and 13H transition under various stress condition. At zero stress the overlap integrals of 11H, 12H, and 13H are in the ratio of 100:0:2. The

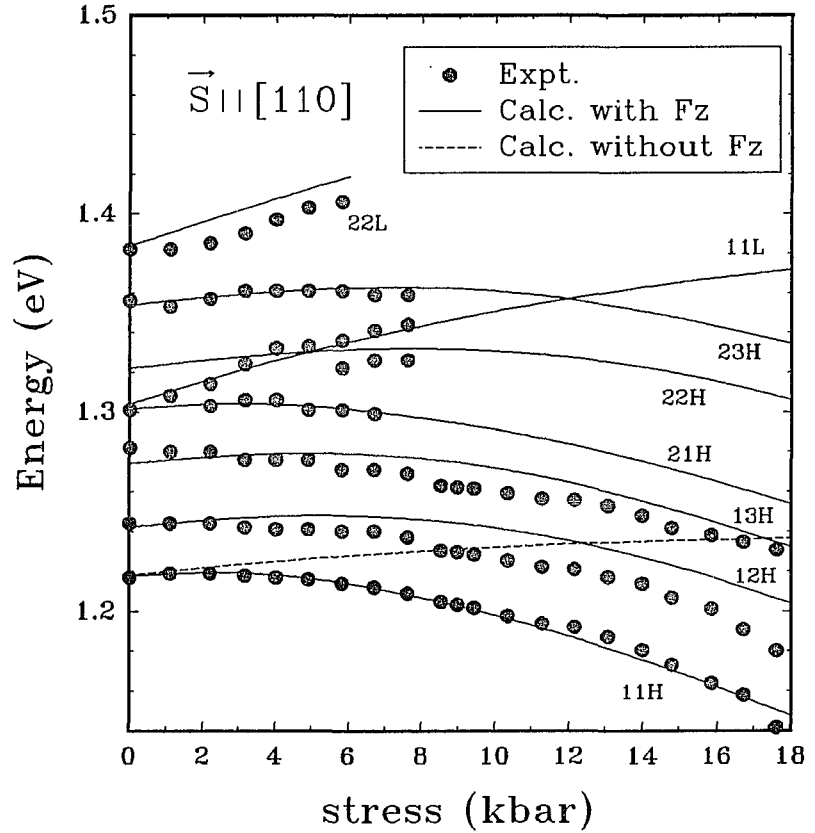


FIG. 57 Stress dependent energies of various quantum transitions in an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW for $S \parallel [110]$.

nonzero amplitude of 13H is a consequence of the finite depth of the well. At about 8 kbar the intensity of 11H has decreased, while 12H has increased so that they are approximately equal. The amplitudes of the three features are now in the ratio 40:40:15. As the stress increases these intensities continue to change so that at $S=18$ kbar we find 7:15:20, i.e., the 13H transition is most intense. This general trend is in good agreement with the data of Figs. 53, 54, and 55.

In conclusion, the influence of large external stress on the energies and intensities of the quantum transitions in a (001) $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW was studied for the

configurations of both $S \parallel [100]$ and $S \parallel [110]$. For the latter case we have observed a significant red shift of 11H, 12H, and 13H as well as a dramatic increase in the intensities of several symmetry forbidden features, an effect not seen for the former stress direction. This phenomenon can be

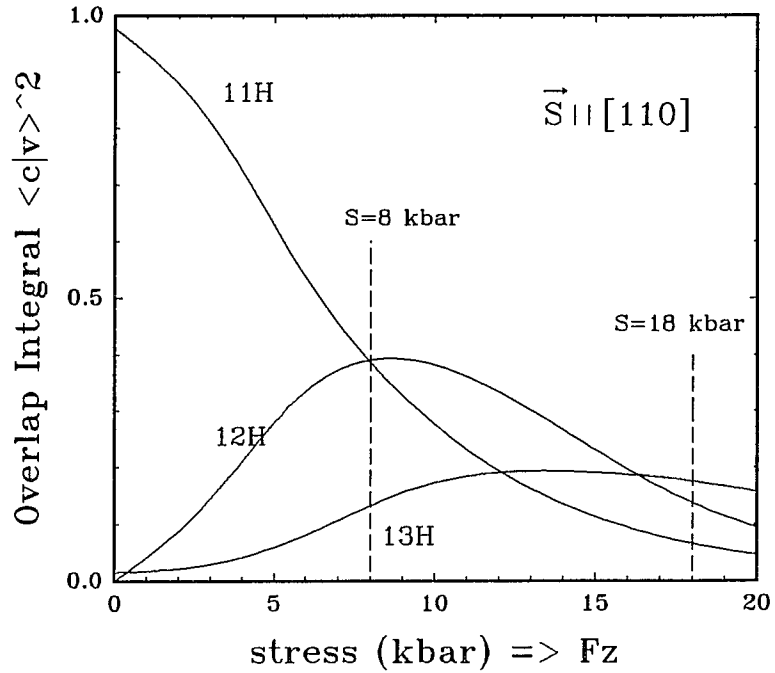


FIG. 58 Calculated stress dependent intensities of 11H, 12H, and 13H transitions in an $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ SQW for $S \parallel [110]$ including piezoelectric effect.

explained in terms of the effect of an electric field generated along $[001]$ due to the piezoelectric coupling for $S \parallel [110]$. A theoretical calculation of the electric field dependence of energies and intensities is in general agreement with the experimental results.

7.3.3 Stress Effects on Lattice Matched GaAs/AlGaAs SQW System

As observed in the previous section, in materials that have strain components $\epsilon_{ij} \neq 0$ ($i \neq j$), there are not only deformation potential effects but also the generation of piezoelectric field. We have carried out a similar study on a (001) GaAs/AlGaAs SQW structure (H. Qiang *et al*, 1992e; F. H. Pollak and H. Qiang, 1992). Measurements

were made for $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$. The $\mathbf{S} \parallel [100]$ results are in agreement on the energy shifts with the early works on GaAs/AlGaAs MQWs although much higher stress range is achieved in this work. In addition, the optical anisotropy (polarization behavior) is observed. For $\mathbf{S} \parallel [110]$ we have observed (a) a red shift of several intersubband features of the SQW, (b) an increase in the intensities of several symmetry forbidden SQW transitions, and (c) FKOs in the signal from the direct gap (E_0) of the AlGaAs barrier layer, while all these are not seen for $\mathbf{S} \parallel [100]$. These electric field related phenomena are again the evidence of piezoelectric coupling presence for this stress direction. However, the magnitude of the electric field associated with the QCSE and FKO is considerably smaller than the piezoelectric field deduced from the piezoelectric coefficients. The observed difference is attributed to the screening mechanism, whose identity is still under further investigation. Also from the stress induced splitting and shifts of the E_0 of $\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ barrier layer for $\mathbf{S} \parallel [100]$ it is possible to evaluate the deformation potentials a and b for this Al composition (see section 7.3.1).

The heterostructure used in this experiment was fabricated by MBE on a (001) semi-insulating GaAs substrate. On top of this was grown 5000Å GaAs buffer, 1000Å AlGaAs, 100Å GaAs (which formed the SQW), 1000Å AlGaAs and 50Å GaAs cap. All are NID layers.

Shown in Fig. 59 by the solid lines are the PR spectra at 300 K for $\mathbf{S}=0$ and $\mathbf{S} \parallel [100]$ (9.7 kbar) for $\mathbf{E} \parallel \mathbf{S}$ and $\mathbf{E} \perp \mathbf{S}$. All the other spectra with intermediate stress

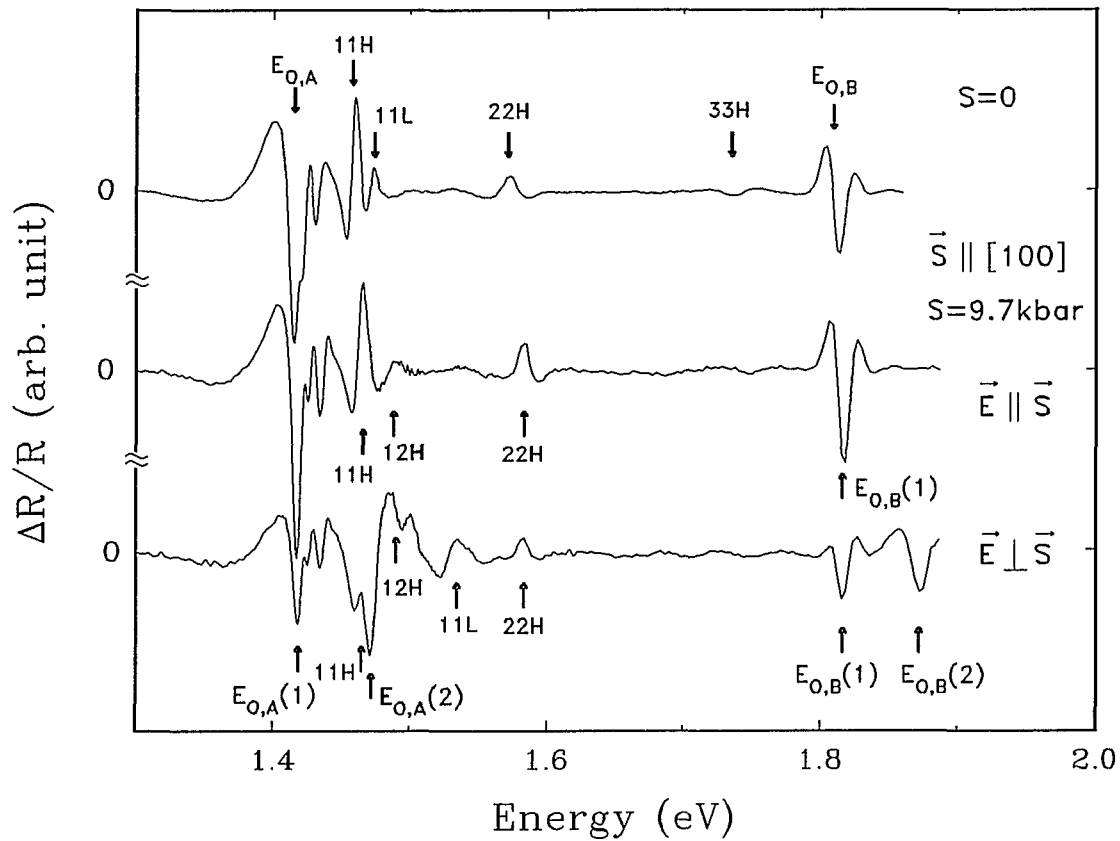


FIG. 59 PR spectra of a GaAs/Al_{0.27}Ga_{0.73}As SQW at 300 K for $S=0$ and $\vec{S} \parallel [100]$ of 9.7 kbar for $\vec{E} \parallel \vec{S}$ and $\vec{E} \perp \vec{S}$.

magnitudes are omitted for simplicity. At $S=0$ the $E_{0,A}$ and $E_{0,B}$ are the E_0 of GaAs and AlGaAs, respectively. From the value of $E_{0,B}=1.810$ eV a 27% Al composition can be deduced. The $E_{0,A}$ trace appears to be a doublet. This is probably due to the fact that the substrate (SI GaAs) and buffer (MBE GaAs) have slightly different gaps. The obtained energies from the least squares fits to an appropriate line shape function are indicated by arrows. The PR trace in the region of the GaAs band gap was too complicated to obtain the energy positions from a reasonable fit and hence the peak position was taken as indicated by the arrow. The main features from the SQW are the symmetry allowed ones, i.e., 11H, 11L, 22H, and 33H.

The 9.7 kbar spectrum for $\mathbf{E} \parallel \mathbf{S}$ appears very much like the $S=0$ data, except that 11L moves out and disappears and a small 12H feature reveals. This is in agreement with previous observations that for this polarization configuration only $E_0(1)$ and HH features in SQW are allowed, both of which have only a small stress dependence. For $\mathbf{E} \perp \mathbf{S}$ the situation is more complicated since besides those appearing in the $\mathbf{E} \parallel \mathbf{S}$ spectrum $E_0(2)$ and mnL features are allowed. The splitting of the valence band of the bulk like material is evident in the AlGaAs features $E_{0,B}(1)$ and $E_{0,B}(2)$. This behavior made it possible to evaluate the deformation potentials a and b for E_0 of this material. The spectrum around $E_{0,A}$ is quite complicated since now the energy of $E_{0,A}(2)$ doublet has shifted into the region of the SQW features. Comparing with the $\mathbf{E} \parallel \mathbf{S}$ spectrum reveals the features of $E_0(2)$ and LH features in SQW. The energies obtained from the line shape fits are indicated by the arrows. It is important to note that there is no appreciable changes in the relative intensities of the various SQW features. All the stress dependence of the energies can be accounted for on the basis of deformation potential theory.

The influence of $\mathbf{S} \parallel [110]$ is quite different. Shown in Fig. 60 are the PR signal at 300 K for $\mathbf{E} \parallel \mathbf{S}$ and $\mathbf{E} \perp \mathbf{S}$ taken at 16.0 kbar. All the signal levels are normalized according to the $S=0$ spectrum. Comparison of $\mathbf{E} \parallel \mathbf{S}$ spectrum with the $\mathbf{S} \parallel [100]$ counterpart shows several dramatic differences that (a) signal levels are higher, (b) FKO appears on the $E_{0,B}(1)$ feature, and (c) several symmetry forbidden transitions like 13H, 21H, and 32H pop up. All these phenomena may be traced back to the electric field

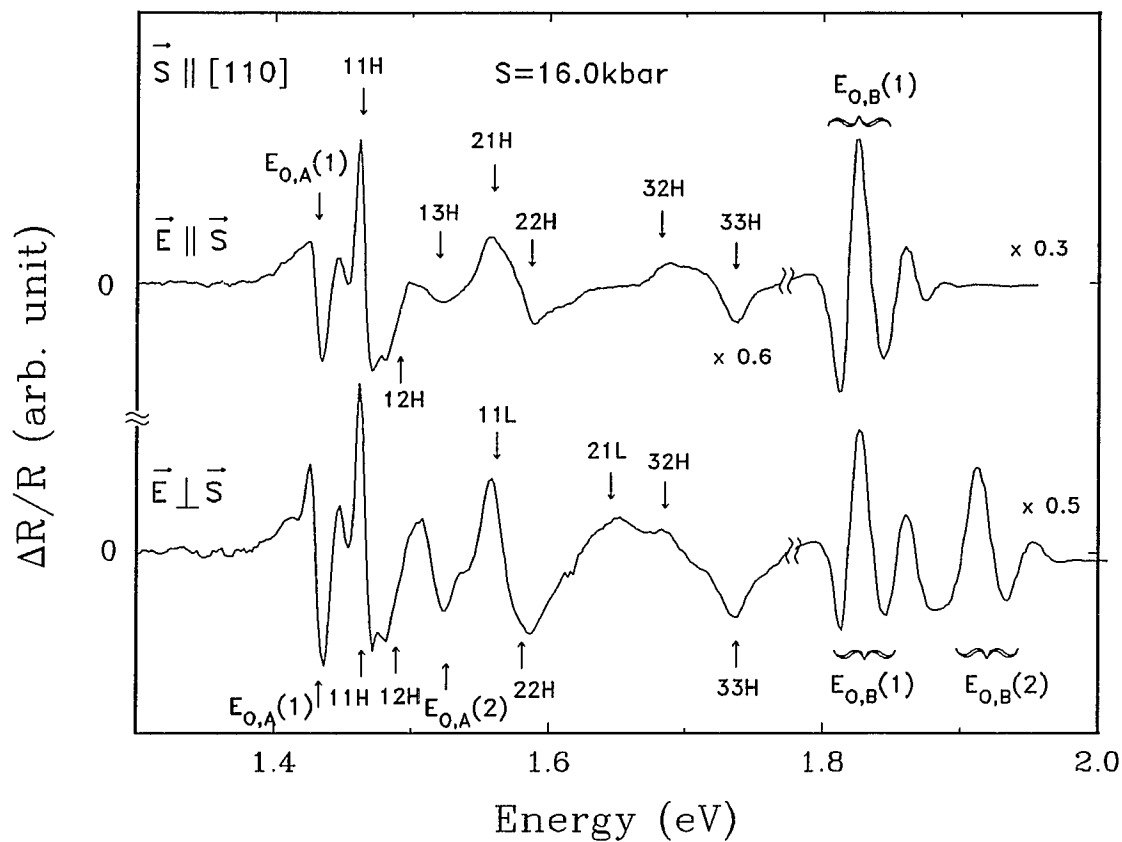


FIG. 60 PR spectra of a GaAs/Al_{0.27}Ga_{0.73}As SQW at 300 K for $S \parallel [110]$ of 16.0 kbar for $E \parallel S$ and $E \perp S$.

generated by piezoelectric coupling. The spectrum for $E \perp S$ is more complicated than $E \parallel S$ because of the appearance of $E_0(2)$ and LH features, but the similar phenomena emerging from the electric field are evident. From the period of the FKO's associated with $E_{0,B}$, a field of 2.6×10^4 V/cm in the AlGaAs region of the sample was determined.

In order to evaluate the QCSE in the SQW for $S \parallel [110]$ the energy difference between 11H and $E_{0,A}(1)$ is displayed in Fig. 61 as a function of applied stress for both $S \parallel [100]$ and $S \parallel [110]$. For the former configuration this difference is almost independent of S , in agreement with a deformation/quantum confinement calculation as shown by the

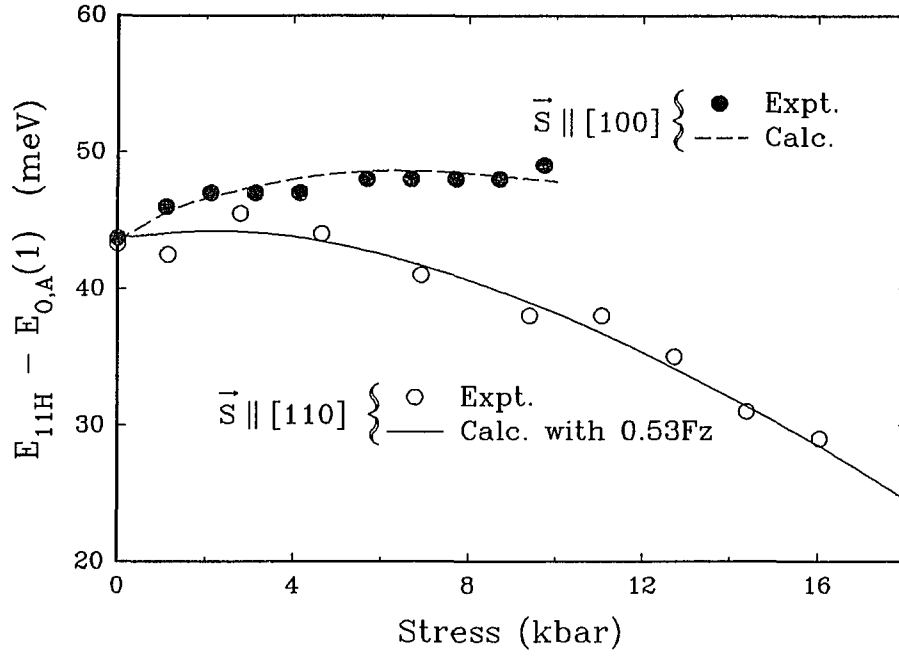


FIG. 61 Stress dependent confinement energies $E_{11H}-E_{0,A}(1)$ of a GaAs/ $\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ SQW for $S \parallel [100]$ and $S \parallel [110]$. Dashed and solid lines are calculations.

dashed line. However, for $S \parallel [110]$ there is an appreciable red shift (i.e., QCSE) of about 17 meV for $S=16.0$ kbar, which corresponds to a field of 9.5×10^4 V/cm. However, for this stress a field of $F_z=1.80 \times 10^5$ V/cm due to piezoelectric coupling is evaluated [see Eq. (7.3)]. Therefore, there must exist some charge states at surfaces (interfaces), or perhaps the bulk AlGaAs, which screens out a large portion of the piezoelectric field.

For example, the difference between the observed and calculated fields at the highest stress can be explained by the presence of free charge equal to $1.1 \times 10^{12} \text{ cm}^{-2}$ at the AlGaAs surface (and back interface) and $5.0 \times 10^{11} \text{ cm}^{-2}$ at the GaAs SQW/AlGaAs interfaces, assuming no background doping, free carriers, etc. Such surface/interface

charge densities are not unreasonable. For example, X. Yin *et al* (1992) have recently determined a density of surface states of $(1.0 \pm 0.6) \times 10^{13} \text{ cm}^{-2}$ on (001) GaAs, which is responsible for pinning of the Fermi level. Meiners (1981) also has reported a surface charge density of about 10^{13} cm^{-2} on (001) semiconductor surfaces. Heterojunction interfaces generally have much lower trap densities in relation to surfaces (D. E. Aspnes, 1983). Duggan *et al* (1992) also have observed the screening of the piezoelectric field by free charges in internally strained (111) InGaAs/GaAs pseudomorphic QWs.

The above discussion has neglected any background doping on trapped charge (T. W. Hickmott *et al*, 1985) in the bulk of AlGaAs. These bulk charges would in general reduce the role of surface/interface states. We have examined another similar GaAs-/AlGaAs SQW structure with a $1 \mu\text{m}$ thick AlGaAs barrier layer on top of the $100 \text{ \AA}$ GaAs QW layer instead of $1000 \text{ \AA}$ here. The observed screening effect was about the same as we discussed here, which suggests the importance of the role of bulk charges. Also the difference of the screening reduction factor on the GaAs/AlGaAs (~ 0.53) and InGaAs/GaAs (~ 1) (see preceding section) SQWs suggests that the presence of the Al may be an important factor in producing the screening effect discussed above. The presence of Al at an interface produces interface states, probably due to gettering of Oxygen by the Al (P. D. Kirchner *et al*, 1981).

If we assume that the piezoelectric field is reduced by a constant screening factor of 0.53 throughout the stress range, we can calculate the predicted red shift due primarily

to the QCSE as shown by the solid line in Fig. 61. There is a good agreement with the experimentally determined values.

We have evaluated the deformation potentials of $\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ material based on its E_0 features. The obtained value of $a=8.6$ eV is substantially smaller than $a=10.7$ eV for $\text{Al}_{0.22}\text{Ga}_{0.78}\text{As}$ discussed in section 6.3.1. This is somewhat surprising. However, these results are consistent with hydrostatic pressure measurements (N. Lipshitz *et al*, 1979) which show a cusp for this parameter for an Al composition of about 27%. On the other hand the value of $b=1.90\pm0.2$ eV shows no such discontinuity with this quantity (2.08 ± 0.2 eV) for the 22% Al sample.

In conclusion, we have investigated the effects of large uniaxial stress along [100] and [110] on the PR spectra at 300 K of a (001) $\text{GaAs}/\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ SQW structure. For $S \parallel [100]$ the stress induced effects in both the SQW and AlGaAs can be explained using only deformation potential theory. From the splitting/shifts of the E_0 of $\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ we have evaluated the hydrostatic and shear deformation potentials for this Al composition. For $S \parallel [110]$ we have observed a QCSE in the SQW and FKO's from E_0 of AlGaAs which enabled us to determine the stress induced fields in these regions. However, the magnitudes of these fields are considerably smaller than deduced from the piezoelectric effect. We have ascribed these differences to surface/interface charge. Thus, the externally tuned piezoelectric effect may be a valuable tool to probe such surface/interface states.

7.3.4 Stress Effects on Biaxially Tensioned GaAs SOW/Si System

The growth of GaAs and GaAs/AlGaAs quantum structures directly on (001) Si is of considerable interest from both a fundamental as well as application point of view. The GaAs/Si structure is under an in-plane biaxial tensile stress arising during post growth cooling from the differences in their thermal expansion coefficients (see for example M. Dutta *et al*, 1990; A. Freundlich *et al*, 1989 and references therein). The structural, electrical, and optical properties of this heterostructure depend strongly on this internal strain. Such strain causes considerable changes in the conduction and valence band structure of the bulk GaAs/Si in addition to GaAs/AlGaAs QWs on the Si substrate (GaAs QW/Si) (C. Jagannath *et al*, 1989; K. Shum *et al*, 1991). For bulk GaAs/Si, the biaxial stress causes a shift and splitting of the fundamental direct band gap (E_0). In such a case, the conduction to out-plane "light-hole-like" (LH) transition [$E_0(2)$] occurs at a lower energy in relation to out-plane "heavy-hole-like" (HH) feature [$E_0(1)$]. In QWs, the ordering of the LH and HH features can be tuned by varying the width of the well (C. Jagannath *et al*, 1989; K. Shum *et al*, 1991). Bulk GaAs/Si has been studied by a variety of optical methods including room (M. Dutta *et al*, 1990) and low temperature PR (A. Freundlich *et al*, 1989). The biaxially stressed excitons in GaAs QW/Si have been investigated by PL, PLE (C. Jagannath *et al*, 1989), and time resolved PL (K. Shum *et al*, 1991) spectroscopy.

We have studied the influence of large external compressive uniaxial stress $S \parallel [100]$ (~ 10 kbar) on the room temperature PR spectra of the built-in strain split direct

gap of (001) GaAs/Si and various quantum transitions of two (001) GaAs QW/Si having different well widths ($L_z=52$ and $200\text{\AA}$) (H. Qiang *et al*, 1992d). For the former, the HH is the ground state, while the reverse is true for the latter. The compressive $S \parallel [100]$ causes a fairly large blue shift of LH transitions since the hydrostatic and shear components of S add, while the HH features are fairly insensitive to the external strain since the two components tend to cancel (F. Pollak, 1990). This property has allowed us to (a) conclusively identify the nature of the observed transitions in both bulk material as well as two SQWs and (b) to tune the LH-HH splitting. For example, in both the bulk material and the $L_z=200\text{\AA}$ sample, it has been possible to make the HH transition the ground state. In addition, because the external strain axis is not collinear with the growth/built-in strain direction, there is an anticrossing of the LH-HH features. This anticrossing produces a very interesting polarization dependence intensity effect which could have important device applications in polarization optical modulators. The tuning of the LH-HH splitting in the SQWs has considerable implications for energy relaxation studies such as those reported by Shum *et al* (1991).

The sample structures were fabricated by MBE on (001) Si substrates tilted by 4° towards (110) by Prof. H. Morkoc's group of University of Illinois at Urbana-Champaign.

The solid curves in Figs. 62 and 63 are the PR spectra for the GaAs SQW/Si sample with $L_z=52\text{\AA}$ for $E \perp S$ and $E \parallel S$, respectively, at different values of $S \parallel [100]$ up

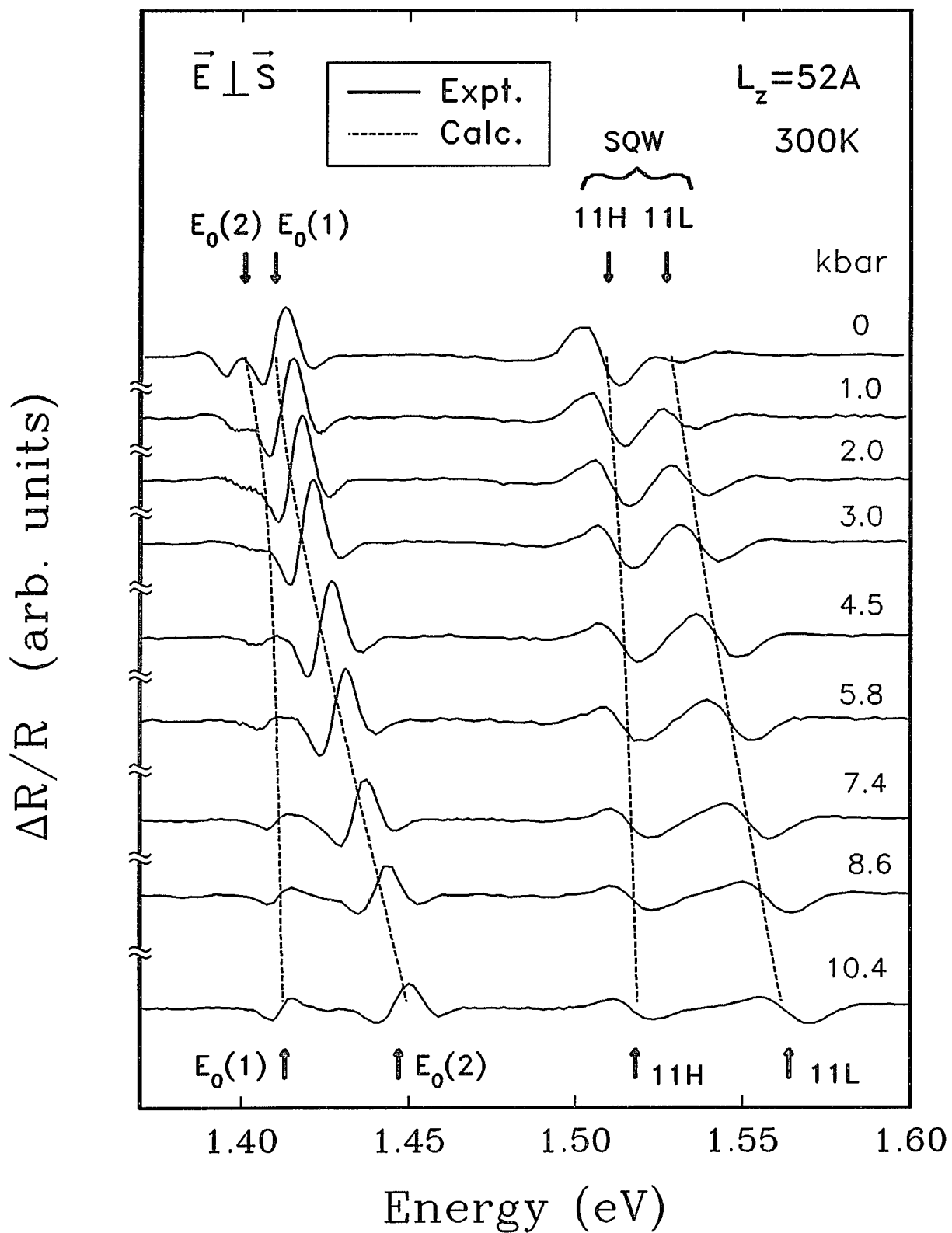


FIG. 62

PR spectra at 300 K for a GaAs SQW/Si ($L_z = 52 \text{ \AA}$) with $S \parallel [100]$ for $E \perp S$.

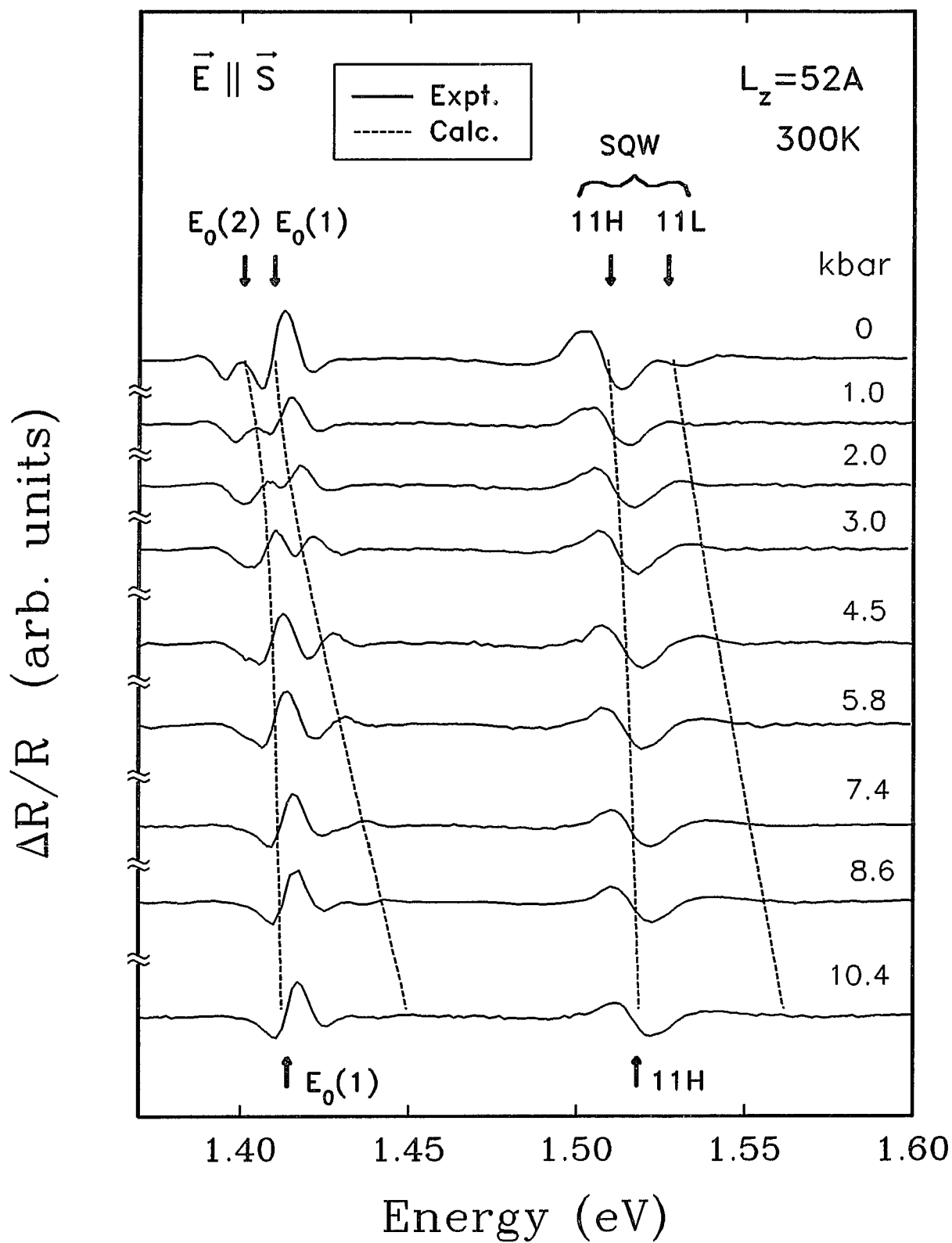


FIG. 63
 $E \parallel S$.

PR spectra at 300 K for a GaAs SQW/Si ($L_z = 52 \text{ \AA}$) with $S \parallel [100]$ for

to 10.4 kbar. Spectra above 10.4 kbar have been omitted because of non-reproducibility associated with the sample, which is probably due to the strain relief effect under high external stress. In the $S=0$ traces, the features around 1.4 eV correspond to the strain split E_0 of bulk GaAs, while the doublet in the vicinity of 1.5 eV corresponds to the 11H and 11L transitions in the SQW. The intensity ratios of 11H:11L and $E_0(1):E_0(2)$ are about 3:1, which is an aid in identifying the transition character nature. Line shape fits to a FDGL function were used to accurately determine the energies and amplitudes of the various spectral features. The line shapes were forced to be identical for a pair of features, i.e., $E_0(2)-E_0(1)$ pair and 11H-11L pair, in order to obtain unambiguous fitting results. This restriction can be justified from both the modulation spectroscopy theory and the experimental observations on the high stress behavior and stress dependence (see Figs. 62 and 63). For clarity, the obtained values of the energies are indicated by arrows only for $S=0$ and 10.4 kbar. Note that at about $S=2.0$ kbar, the intensity of the lower lying E_0 is zero for $E \perp S$ and that at the highest stress (10.4 kbar), the intensities of $E_0(2)$ and 11L are larger than their HH counterparts.

A theoretical calculation of the effects of both internal and external strains were performed on (a) the energy positions of E_0 of bulk GaAs and the quantum transitions of SQWs and (b) the polarization dependence intensities of various transitions. The influence of the spin-orbit-split band was included implicitly (see Chapter 4). The results of this computation for the energy positions are shown by the dashed lines in Figs. 62 and 63. At $S=0$, the $E_0(2)$ feature lies below $E_0(1)$ because of the built-in biaxial tensile

strain, while for this narrow SQW the large quantum confinement effect causes 11L to occur above 11H. The 30% Al composition in the barrier material is confirmed from the separation of E_0 peaks of AlGaAs and GaAs portions. From the $E_0(1)$ - $E_0(2)$ splitting at $S=0$ (9.0 meV) we can evaluate the built-in strain (stress) at 300 K to be -1.2×10^{-3} (1.5 kbar), in support of the previous results (M. Dutta *et al*, 1990; C. Jagannath *et al*, 1989). Including the effects of this built-in strain and using $Q_c=0.65$ before the strain effects, the best fit to the observed 11H and 11L confinement energies is achieved for $L_z=52$ Å. All the structure parameters are thus determined. The influence of the external stress is to cause a blue shift of $E_0(2)$ and 11L while the $E_0(1)$ and 11H features remain relatively insensitive to S . At the highest stress $E_0(2)$ lies above $E_0(1)$ while for the SQW the HH-LH splitting has been substantially increased. There is good agreement between the theoretical calculation and the experimental results.

For the E_0 transitions there is actually a strong anticrossing of the LH and HH peaks at about 2 kbar due to the fact that S is not collinear with the growth/built-in strain axis. Similar (but much smaller) LH-HH anticrossings have been observed for certain transitions (e.g., 11L-13H) in GaAs/AlGaAs MQWs under similar stress configurations (F. Pollak, 1990 and references therein). This anticrossing also produces a very interesting polarization effect which has not previously been reported. Plotted in Fig. 64 are the calculated intensities of the E_0 transitions as a function of S (including the built-in strain) for $E \perp S$ (solid line) and $E \parallel S$ (dashed line). The intensity is given by the conduction and strain dependent valence band wavefunction overlap integral. At

$S=0$, the intensities of $E_0(2)$ and $E_0(1)$ are in the ratio of 1:3, in agreement with the experimental data in Figs. 62 and 63.

At a value of $S \approx 2.4$ kbar for

$\vec{E} \perp \vec{S}$, the intensity of the features that

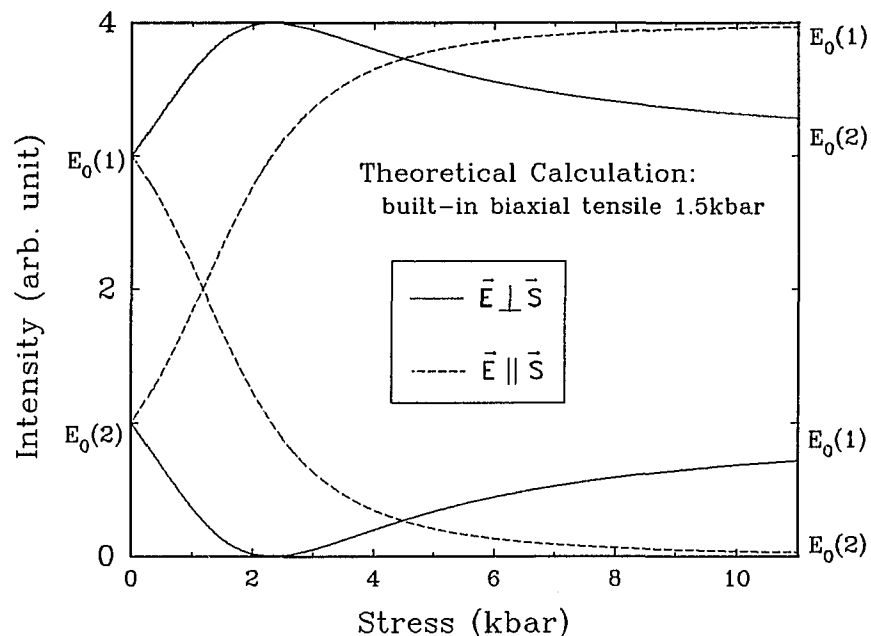


FIG. 64 Calculated stress dependence of the E_0 intensities of bulk GaAs/Si for $\vec{S} \parallel [100]$ at 300 K.

started as $E_0(2)$ and $E_0(1)$ are zero and maximum, respectively. This is a consequence of the anticrossing. Note that in Fig. 62, the intensity of the lowest lying feature is zero. It should be noted that in this anticrossing region the designation of $E_0(2)$ and $E_0(1)$ would be rather ambiguous because of the strong LH-HH coupling. At the highest stress (10.4 kbar) $E_0(2)$ for $\vec{E} \parallel \vec{S}$ is essentially zero, while for $\vec{E} \perp \vec{S}$ the ratio of $E_0(1):E_0(2)$ is approaching 1:3. This implies that the contribution of built-in strain becomes negligible at high enough external stress so that all behaviors will eventually approach that of a plain bulk material (see Fig. 45). Furthermore, at the highest strain similar intensity effects should apply for 11H and 11L. These results are in good agreement with the data displayed in Figs. 62 and 63.

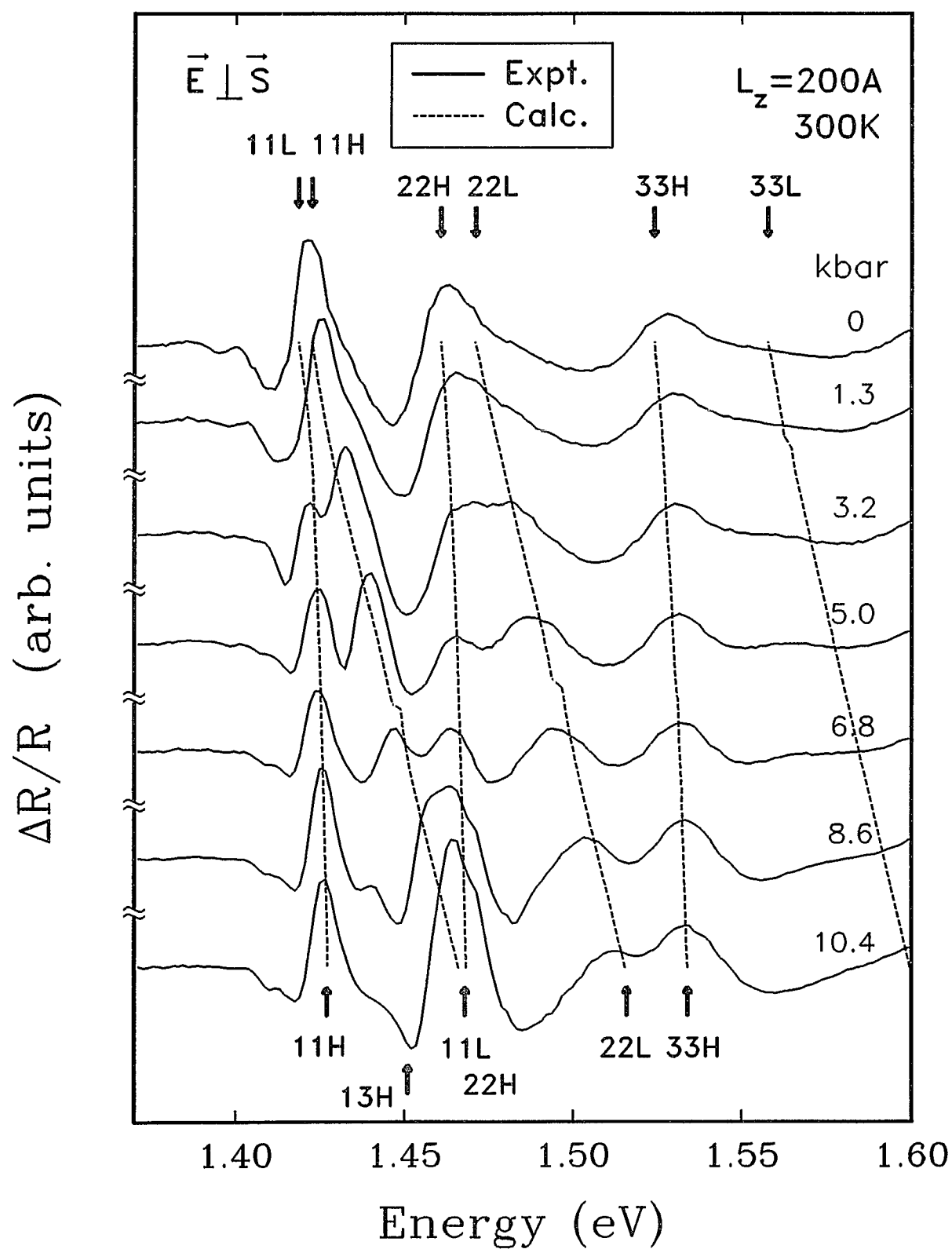


FIG. 65
 $\vec{E} \perp \vec{S}$.

PR spectra at 300 K for a GaAs SQW/Si ($L_z = 200 \text{ \AA}$) with $\vec{S} \parallel [100]$ for

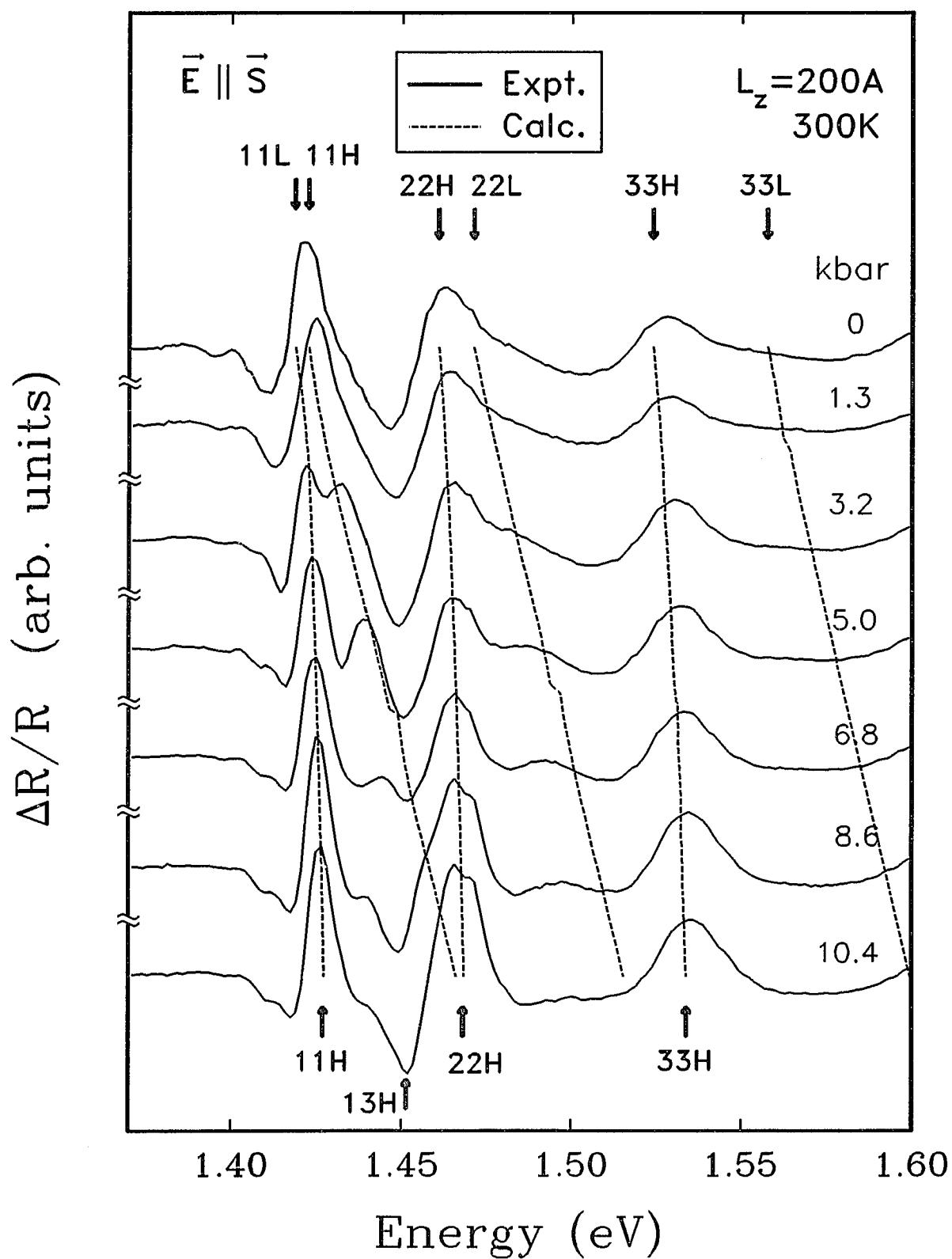


FIG. 66
 $\vec{E} \parallel \vec{S}$.

PR spectra at 300 K for a GaAs SQW/Si ($L_z = 200 \text{ \AA}$) with $\vec{S} \parallel [100]$ for

In Figs. 65 and 66 are plots of the results of 200 Å SQW for various values of S for $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$, respectively. We show the spectra of stress up to 10.4 kbar in consistency with that of the 52 Å sample, although the higher stress spectra are quite reproducible for this sample. For this sample E_0 singals of GaAs are very weak and hence we will concentrate on the SQW transitions. Again we show the obtained energy positions from line shape fits by the arrows for $S=0$ and 10.4 kbar, and the dashed lines are the theoretical calculations. At $S=0$ the 11L feature lies below 11H although these peaks as well as 22H-22L are not resolved at 300K. The ordering has been identified from the backtracking of the S dependence and from a PR measurement at 77 K, where the features are resolved. The detailed results at 77 K will be discussed latter. At about 1 kbar there is an anticrossing of 11L and 11H. Note that at $S=3.2$ kbar two peaks are clearly visible in the region of 11L-11H and 22H-22L. Furthermore, at the highest stress shown here the intensities of the LH features for $\mathbf{E} \parallel \mathbf{S}$ are essentially zero, in agreement with Fig. 64.

Displayed by the solid lines in Figs. 67 and 68 are the PR spectra at 77 K of the $L_z=200\text{\AA}$ sample for different values of $S \parallel [100]$ with $\mathbf{E} \perp \mathbf{S}$ and $\mathbf{E} \parallel \mathbf{S}$, respectively. The lowering of sample temperature affects the PR spectra in two ways. First, the linewidth of various features are narrower due to less thermal broadening so that the spectral resolution is much better. Secondly, further cooling introduces more built-in biaxial tensile strain on the III-V material layers due to different thermal expansion coefficients with Si substrate, which increases the 11L-11H separation. These two effects are evident

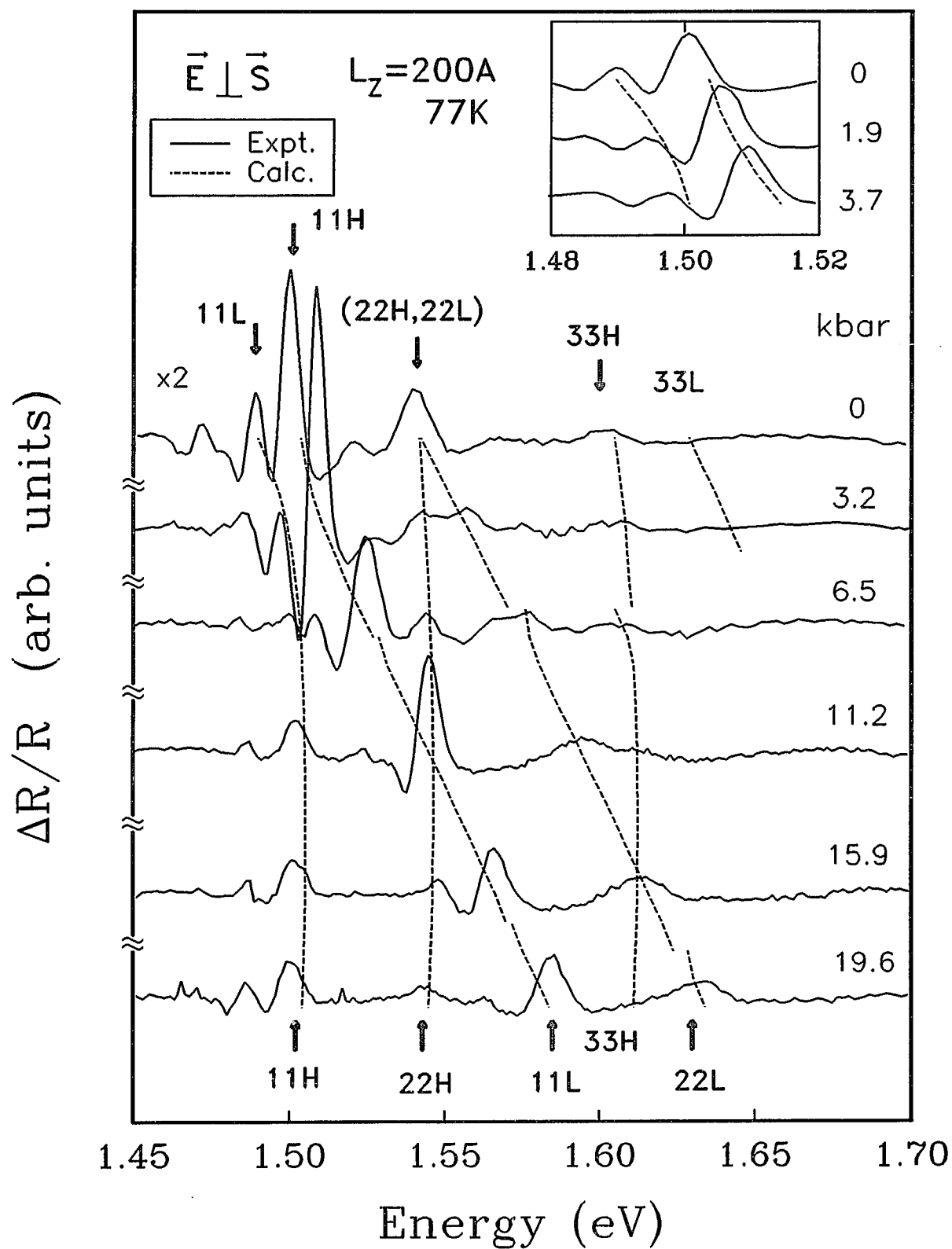


FIG. 67

PR spectra at 77 K for a GaAs SQW/Si ($L_z = 200 \text{ \AA}$) with $S \parallel [100]$ for $E \perp S$.

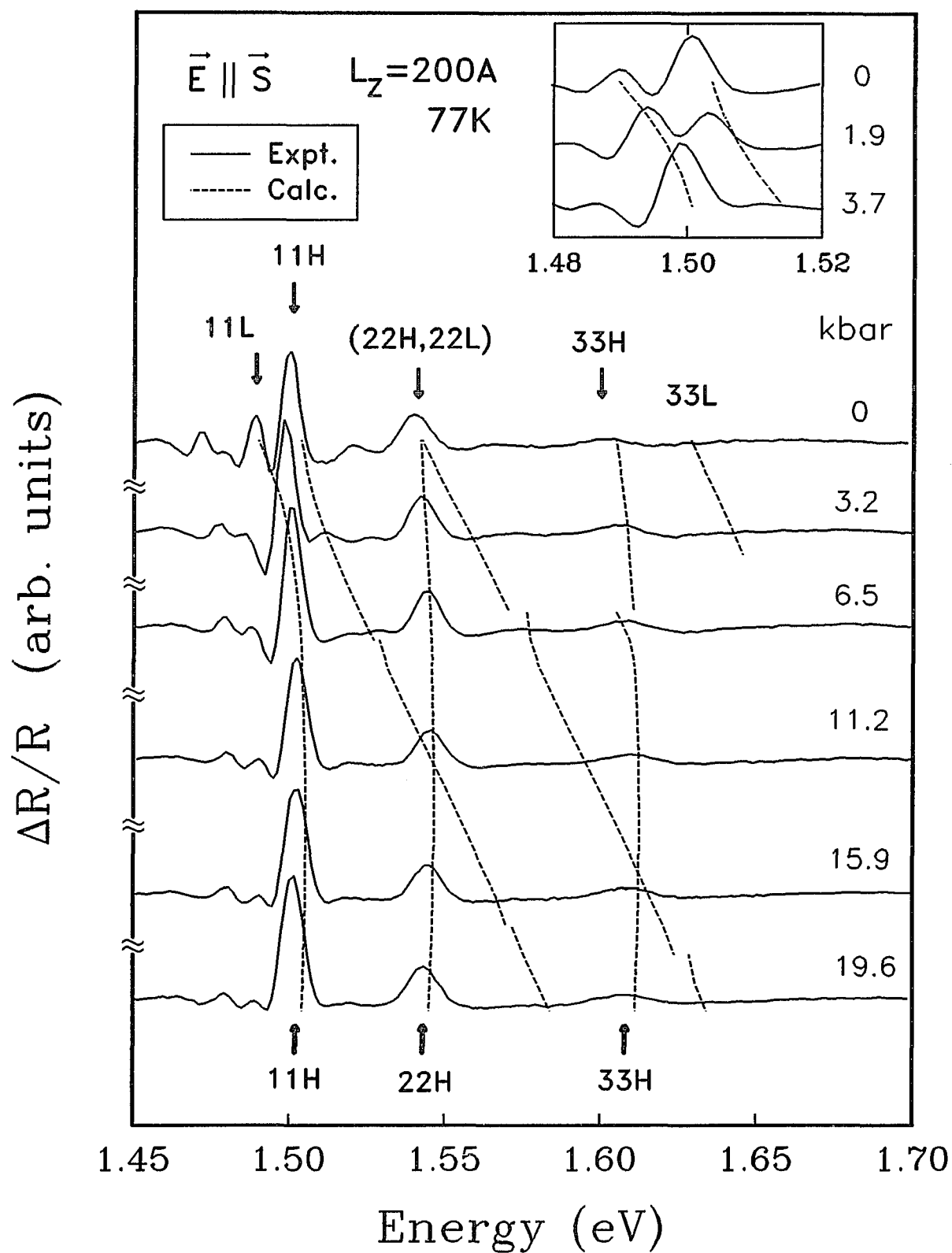


FIG. 68
 $\vec{E} \parallel \vec{S}$.

PR spectra at 77 K for a GaAs SQW/Si ($L_z = 200 \text{ \AA}$) with $\vec{S} \parallel [100]$ for

if we compare the 77K spectra with the corresponding 300K spectra. At $S=0$, the well resolved features of 11L and 11H enable us to determine a built-in biaxial stress of 2.5 kbar at 77K. Using this value, we did the same calculation as at 300K. The results are shown in the Figs. 67 and 68 as dashed lines. They are again in good agreement with the experimental observed features. The familiar stress dependence of LH features are observed, i.e., strong dependence of energy positions and disappearing intensity for $E \parallel S$. Also note the lower energy side of 11H and 11L features. The weak signals due to $E_0(1)$ and $E_0(2)$ of GaAs are now resolved and they have similar energy and polarization dependent intensity changes as the related 11H and 11L peaks. Since 11L lies below 11H at $S=0$ and will move to high energy side of 11H at high stress, we expect to see an anticrossing behavior similar to that of E_0 of bulk GaAs/Si. This is indeed the situation around $S=2.0$ kbar. Shown in the insets of Figs. 67 and 68 are the enlarged portions of PR spectra near 11L-11H region for $S=0$, 1.9, and 3.7 kbar. The observed dramatic energy and polarization dependent intensity changes are to be compared with those of GaAs E_0 features in Figs. 62 and 63. Thus, it is clear that the ordering of fundamental LH and HH transitions in the 200Å GaAs SQW/Si is the same as bulk GaAs/Si while opposite to the 52Å GaAs SQW/Si.

In conclusion, we have studied the effects of large, external $S \parallel [100]$ on the optical features of two GaAs microstructures fabricated on (001) Si, including polarization effects. The observed stress dependent energy shifts are in good agreement with a theoretical calculation, which has made it possible to conclusively identify the

nature of the observed transitions in both bulk GaAs and two SQWs. In addition, the strong anticrossing of the LH-HH features in the bulk material produces an interesting polarization effect which also has been accounted for by our theory. The ability to tune the LH-HH splitting in quantum wells has considerable applications for time dependent PL studies, which will be discussed in the following chapter.

7.3.5 Growth Directional Stress $\vec{S} \parallel [001]$ on GaAs/AlGaAs SQW

A growth direction-al stress setup has been developed. This is a complementary configuration to the in-plane stress situations. This is a simpler stress configuration since the HH and LH band are decoupled at $k_x = k_y = 0$. But it is more difficult to implement experimentally because of the thin film layer form of the semiconductor microstructure samples. Previous works

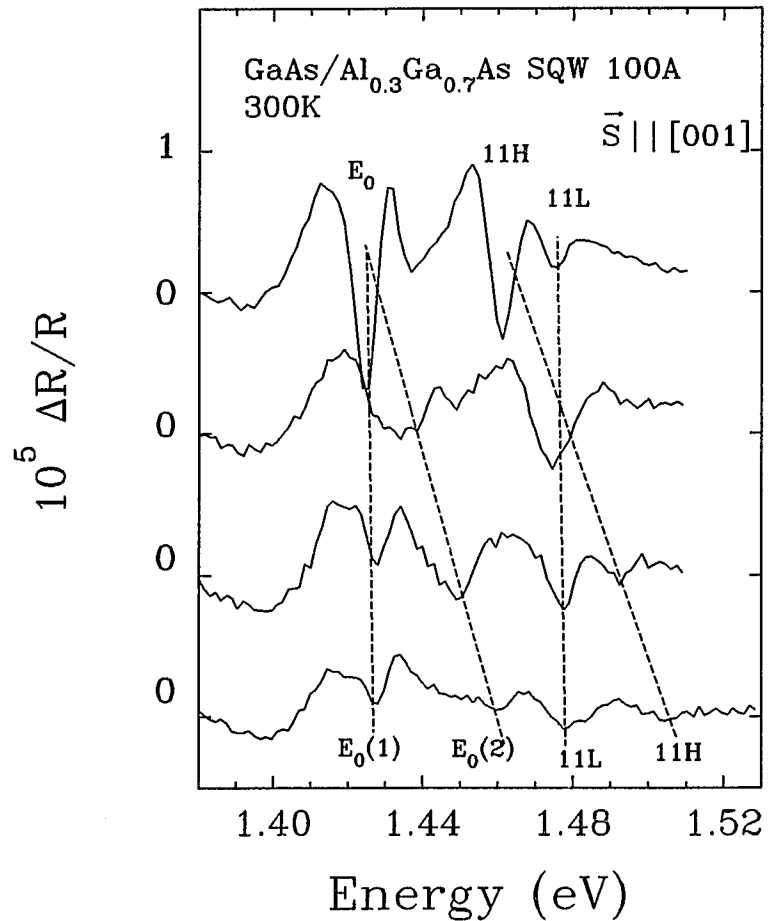


FIG. 69 PR spectra (solid lines) of a GaAs/AlGaAs SQW at 300K for $\vec{S} \parallel [001]$. The dashed lines are drawn as guide to eyes.

have reported only about 3 kbar maximum stress for $S \parallel [001]$ (P. Lefebvre *et al*, 1989).

We have modified our stress apparatus to include this configuration. Some very preliminary testing results are very encouraging. Shown in Fig. 69 as solid lines are PR spectra taken at room temperature on a GaAs/AlGaAs SQW structure with different stress. The dashed lines are drawn as guide lines to the eyes. Although the experimental conditions are not optimized so that the signal is noisy, the stress induced changes of the energy positions are quite clear on both the E_0 feature of GaAs substrate and the quantum transitions of the QW region. In this configuration the 11H has larger stress dependence than the 11L feature. The non-resonant cross over of the two features are observed. The stress dependence is different from the $S \parallel [100]$ configuration (see Fig. 59). The observed energy shift of 11H is almost 50meV, which corresponds to about 8 kbar applicable stress. Thus large uniaxial stress is possible along the growth direction. We do not observe a significant broadening changes on the quantum transitions and the spectrum is well reproduced after the stress is released. Therefore, the well defined elastic strain distribution is obtained on the sample.

This preliminary experimental result shows that the growth directional uniaxial stress can be achieved on wafered sample with significantly higher magnitude while maintain a homogeneous elastic strain distribution. This simpler stress configuration will enable us to do various research work with better defined band structures. For example, the influence of the Γ -X resonance on the carrier dynamics can be studied.

7.4 Summary

Uniaxial stress is a valuable tool in probing and tuning the electronic band structures of semiconductor microstructures, while relatively few works were reported in this study. Its influence can be readily explained in the context of deformation potential theory. For a III-V Zinc-blend type material, three material parameters are involved, i.e, a (hydrostatic deformation), b (Tetragonal deformation), and d (Trihedral deformation). Our work has benefitted from the relative high available stress magnitude of our uniaxial stress setup. The results of this work are summarized as:

- Measurements of deformation potentials of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ternary materials are shown in Table X for several Al compositions. A discontinuity of the parameters around 0.22-0.27 is suggested from the table. This issue needs further investigation.
- In-plane uniaxial stress $S \parallel [100]$ is studied on the SQWs of various material systems including InGaAs/GaAs, GaAs/AlGaAs, and GaAs/AlGaAs grown on Si substrate, in which the built-in biaxial stress is compressive, zero, and tensile, respectively.
 - (a) The experimental behaviors are well pictured by the quantum confinement effect together with the band mixing described by deformation potential theory including the interaction with spin-orbit-split band.
 - (b) The HH/LH features have small/large stress dependence. Features of the

same character have about the same quantitative stress dependence. This makes it possible to tune the electronic band structures by external uniaxial stress.

- (c) The LH features have strong polarization dependence at high stress. They can only be observed for $\mathbf{E} \parallel \mathbf{S}$, while the HH features have usually weaker intensities for $\mathbf{E} \perp \mathbf{S}$ than $\mathbf{E} \parallel \mathbf{S}$. This polarization behavior together with the different stress dependence of energy positions make it a powerful tool in identifying the character nature of various optical features.
 - (d) The intensities of various transitions are insensitive to the external uniaxial stress. The symmetry allowed transitions dominate the spectra across the stress range.
 - (e) In biaxially tensile stressed material system, e.g., GaAs SQW/Si, the fundamental transition has an out-plane LH character if the well width is large enough. In these systems, since the LH features have bigger stress dependence, the ground state will eventually be HH transition at high stress. At the cross-over stress position, a strong anticrossing between these two levels was observed, which shows interesting polarization behavior.
- In-plane uniaxial stress $\mathbf{S} \parallel [110]$ is also studied on the SQWs of various material systems including InGaAs/GaAs and GaAs/AlGaAs. Several effects due to piezoelectric field, such as QCSE and FKO, are observed. They are:

- (a) The PR signal level of the spectra increases with stress, which is due to the increased modulation because of the increased built-in electric field.
 - (b) Besides the different stress dependence of energy positions between HH and LH, extra red shifts of the strong HH features are observed.
 - (c) The relative intensities change with stress. The "symmetry-forbidden" transitions become more and more intense as compared to the "symmetry-allowed" transitions.
 - (d) The FKO features around the barrier material signals emerge with the stress.
 - (e) In order to account for the observed QCSE of the SQW features, we need a 100% (53%) of calculated piezoelectric field in the InGaAs/GaAs (GaAs/AlGaAs) SQW. The different screening factors between the two system need further investigation. The presence of the Al may contribute to certain extent.
- A growth directional uniaxial stress apparatus has been developed. The preliminary result is encouraging. We show that about 8 kbar stress can be achieved on thin film samples.

Chapter 8. Uniaxial Stress Effect -Dynamic Properties

8.1 Introduction

In previous chapter, we show that uniaxial stress can bring about structural change which causes dramatic change to the electronic band structures. Because of these changes in the material and the changes of the inter-band and intra-band matrix elements as well as the change of phonon dispersion curves, the dynamic properties are also expected to undergo dramatic changes.

In collaboration with the Institute for Ultrafast Spectroscopy and Lasers of the City College of New York, we have carried out systematic studies on several semiconductor materials and semiconductor microstructures under the influence of larger external uniaxial stress.

Stress induced changes of hole dynamic properties have been studied on a bulk n^+ -GaAs material. The results will be discussed in section 8.3.1.

We have seen in the previous chapter that uniaxial stress can continuously tune the band structures of semiconductor microstructures including the HH and LH subband ordering. We have carried out time-resolved PL studies on GaAs QW/Si structures of both intrinsic and p^+ doped materials. The intrinsic sample of 200Å GaAs SQW/Si structure is the same as the one discussed in section 7.3.4. The non-intensional doping

level of this material enables us to examine the exciton dynamic property changes under in-plane uniaxial stress. The results will be discussed in section 8.3.2. Another similar structure of 188Å GaAs MQW/Si has initial p^+ doping, which enables us to examine the changes of free carrier dynamics. The Be dopants are all placed in the middle of the barrier regions in order to eliminate the impurity centers inside the well regions. The results of this modulation doped MQW structure will be discussed in section 8.3.3.

8.2 Experimental Setup

The uniaxial stress setup has been described in the previous section. The low temperature is achieved on a Janis DT-80 dual cooling dewar. Although temperature control is possible, it is not used. The excellent temperature stability is ensured by keeping enough liquid Helium flow, in particular, some experiments were performed with sample emerged in the liquid Helium which is kept below the λ point by maintaining a low pressure environment.

The dynamic properties are studied by the picosecond time-resolved PL spectroscopy using a synchroscan streak camera with 10 ps time resolution. The photoexcitation is by 2.0 eV, 100 fs CPM laser pulses generated from a colliding pulse mode-locked ring dye laser. The PL signal from the sample is dispersed by a quarter meter spectrometer (energy dispersion) onto an input slit of the streak camera (time dispersion) so that a three dimensional time and energy resolved PL spectrum can be displayed.

8.3 Experimental Results

8.3.1 Hole Relaxation in n^+ -bulk GaAs

Using the time resolved PL equipment, we have examined the n^+ -GaAs (10^{18} cm^{-3} doping) bulk material under uniaxial stress at 100K (S. Lee *et al*, 1992). The pump beam is a 100fs 620nm CPM laser pulse. The PL signal is simultaneously resolved in both the energy (spectrometer) and time (streak camera) domains.

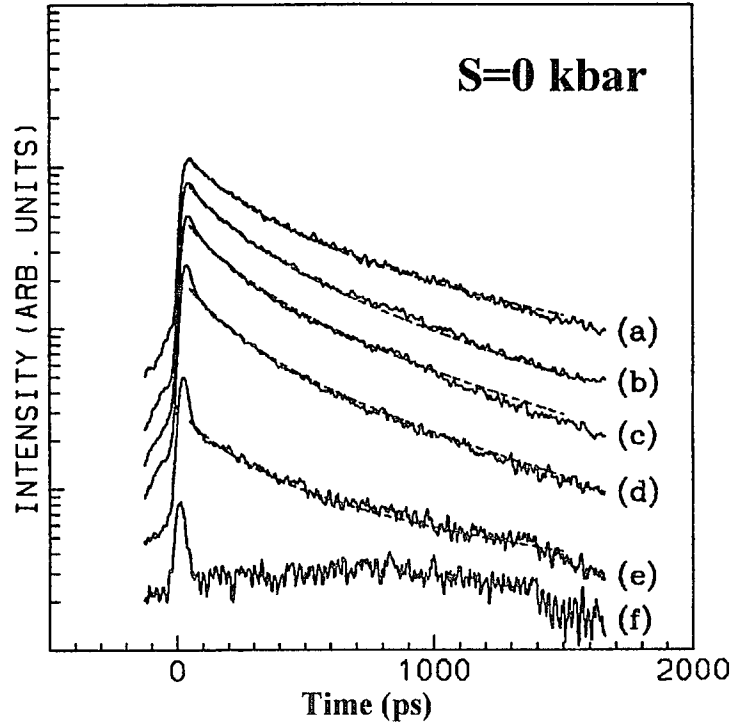


FIG. 70 Time resolved PL spectra of a n^+ -GaAs sample ($S=0$) for 10meV slices at (a)1.48, (b)1.50, (c)1.52, (d)1.54, (e)1.56, and (f)1.58 eV.

Besides the stress dependent transition energies which can be observed from the energy domain, the time resolved spectra reveal the dynamical property changes such as the carrier photo-generation efficiency and the hole lifetimes.

At $S=0$, the PL spectra of several different energy slices are shown in Fig. 70 as solid lines. In our sample the electron density $n(t) \approx n_i$ is due to the high doping concentration. Thus, the major contribution to the relaxation behavior is from the

photogenerated holes. Keeping up to second order process, the relaxation of the hole carrier densities, $p(t)$, is given by:

$$\frac{dp(t)}{dt} = -Ap(t) - Bp^2(t) \quad (8.1)$$

where A is the normal exponential decay constant including both radiative and non-radiative contributions, and B is the bimolecular recombination coefficient.

The analytical solution of this equation is given by:

$$p(t) = \frac{p_0}{(1+u)e^{At} - u} \quad (8.2)$$

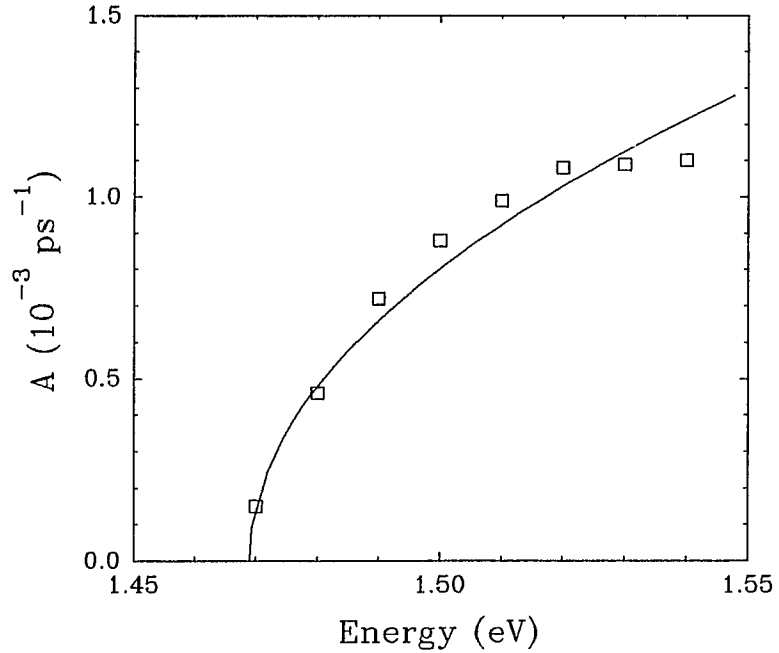
where p_0 is the initial hole density at $t=0$ and u is defined as:

$$u = \frac{Bp_0}{A} \quad (8.3)$$

It can be seen that at the limit of $u \ll 1$ (or $Bp_0 \ll A$), when the bimolecular contribution is negligible, this solution reduces to the regular single exponential decay situation.

The least squares fits of this expression to the experimental time resolved PL traces are shown as the dashed lines in Fig. 70. The satisfactory fitting yields two relaxation coefficients, A , and B , in addition to the initial densities of photogenerated holes

p_0 . The decay constant A is energy dependent below 1.5eV, while relatively stable above it. The experimental determined decay constants A , which are averaged over 10meV energy slices, are displayed in Fig. 71 as



squares against the energy positions. The quantitative energy dependence of

FIG. 71 Decay constant A (squares) as a function of the transition energy. The solid line is a least squares fit to the 3D square root joint density of states distribution function.

A is found to be proportional to the joint density of states distribution. The solid line in the same figure is a fit to the 3D square root density of states function without considering the impurity tail. The decay constant B is independent of energy.

The uniaxial stress was applied along $\mathbf{S} \parallel [100]$ to examine the changes on these relaxation parameters. Studies of ν_1 band are carried out on the $\mathbf{E} \parallel \mathbf{S}$ spectra where only $E_0(1)$ is allowed, since for $\mathbf{E} \perp \mathbf{S}$ the presence of both $E_0(1)$ and $E_0(2)$ features makes the situation much more complicated and information more subtle. In Figs. 72, 73, and 74, we show as squares the experimentally determined stress dependence of p_0 , A , and B for $\mathbf{E} \parallel \mathbf{S}$, respectively. Plotted are the relative changes normalized to the $S=0$ values.

As shown in Fig. 72, the p_0 increases monotonically with the applied stress. This behavior has been explained due to a stress dependent absorption coefficient. The application of a uniaxial stress changes the effective masses of both conduction and valence bands.

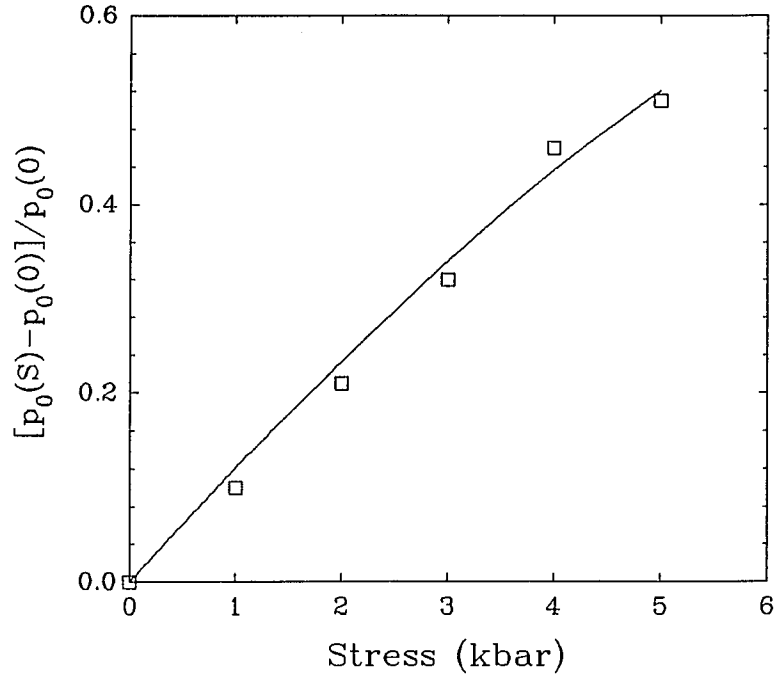


FIG. 72 Relative changes of p_0 due to $S \parallel [100]$ for $E \parallel S$ from both the time resolved PL experiments (squares) and a theoretical calculation (solid line).

This change effectively

modifies the joint density of states, on which the absorption coefficient directly relies. The solid line in Fig. 72 is the calculated change due to stress dependent joint density of states (S. Lee *et al*, 1992), which agrees very well with experimental results.

The decay constant A is weakly dependent on the stress as shown in Fig. 73. Plotted in the figure as squares are the relative changes of A from its $S=0$ value determined from the time resolved spectra. The observed small linear increase has been attributed to the stress dependent matrix element M_{cv} of a dipole oscillator. This matrix element of the $E_0(1)$ transition for $E \parallel S$ depends on the external uniaxial stress by the following expression (see for example F. H. Pollak, 1990):

$$A(S) \propto M_{cv}(S) = \left| \langle c | \hat{e} \cdot \vec{p} | v \rangle \right|^2 = 4P_0^2 \left(1 + \frac{\delta E_{100}(S)}{\Delta_0} \right) \quad (8.4)$$

The solid line in Fig. 73 is the calculation using the experimentally determined deformation potentials of GaAs as discussed in the section 6.3.1. A good agreement to the experimental data can be seen.

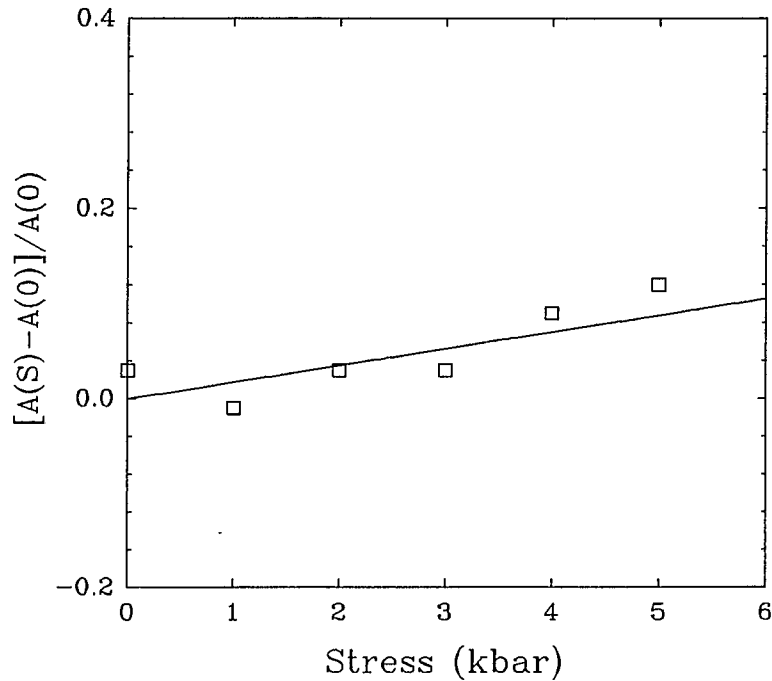


FIG. 73 Relative changes of A due to $S \parallel [100]$ for $E \parallel S$ of both the time resolved PL experiments (squares) and a theoretical calculation (solid line) as explained in the text.

The stress dependence of higher order processes is beyond our

experimental resolution. This is evident by the relative change of bimolecular recombination parameter B shown in Fig. 74 (squares). Note the large data scattering. Although no quantitative dependence can be extracted out of the experimental error bars, a quantitative estimation of the upper limit of stress dependence can be given as $|\Delta B/B| < 2\% \text{ kbar}^{-1}$. We draw two dashed lines of this slope in the same figure as a reference guide to the eyes.

According to their dependence on the carrier density p , the three relaxation parameters can be treated as zero order (p_0), 1st order (A), and 2nd order (B) processes. The linear stress dependence coefficients of the relative changes of these parameters are listed in Table XI. As we see, the stress dependence decreases in

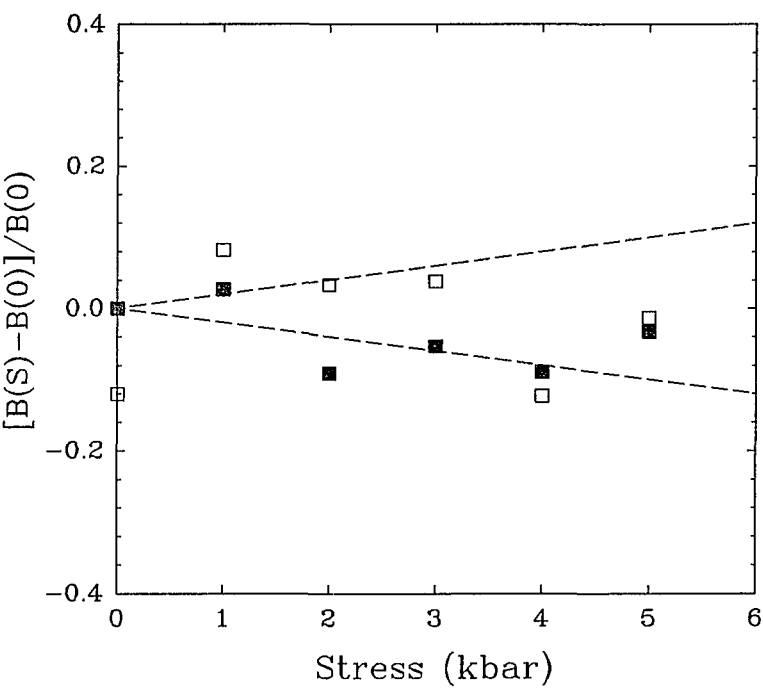


FIG. 74 Relative changes of B due to $S \parallel [100]$ for $E \parallel S$ from the time resolved PL experiments (squares). The dashed lines are the upper limit estimates of stress dependence.

going from zero order process to higher order processes. Based on this trend, we predict that the higher order relaxation processes, e.g., phonon assisted Auger process, will be

much less dependent on stress so that it is negligible within the current stress magnitude.

Table XI Stress dependence of relaxation parameters p_0 , A , and B of a bulk n^+ -GaAs.

relaxation constant	process order	stress dependence of relative change ($10^{-3} \text{ kbar}^{-1}$)
p_0	0th order	107 ± 8
A	1st order	19 ± 6
B	2nd order	< 20

The carrier lifetime is a convenient relaxation

parameter. In an exponential decay situation, $\tau=1/A$. However, since the relaxation process is nonexponential in our sample, the hole lifetime is time dependent. An effective lifetime τ is introduced for this system, which is defined as the time duration when $p(\tau)/p_0=1/e$. It can be

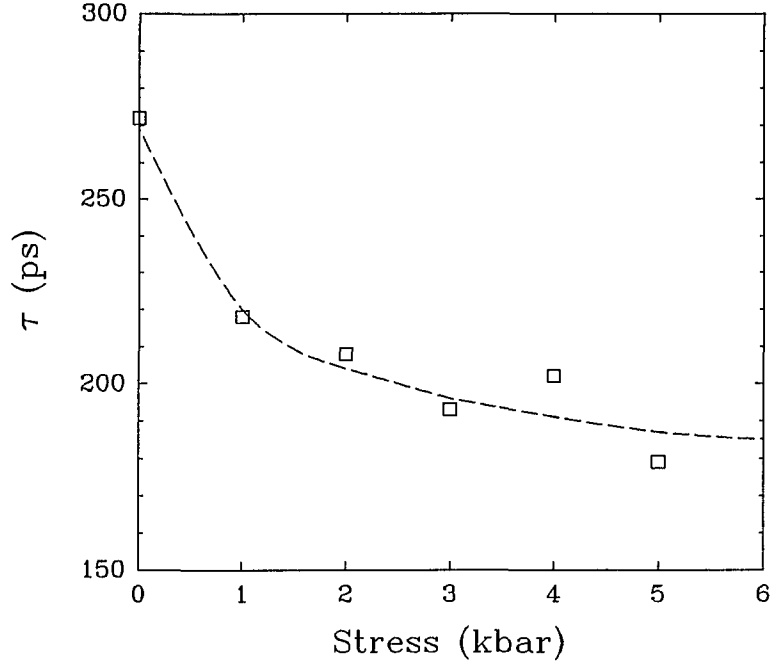


FIG. 75 Stress dependence of effective hole lifetime determined from experiments (squares). The dashed line is a least squares fit to a phenomenological equation (see text).

shown that this effective lifetime is related to the nonexponential relaxation parameters as:

$$\tau(S) = \frac{1}{A} \ln \left[\frac{u+e}{u+1} \right] \quad (8.5)$$

This equation will reduce to the exponential decay situation, $\tau=1/A$, when the low excitation condition, $u \ll 1$ (or $p_0 \ll A/B$), is met. The calculated effective hole lifetimes of our n^+ -GaAs sample are displayed as squares in Fig. 75 with respect to the external uniaxial stress. A reduced lifetime is observed with the increasing stress magnitude. There is a significant reduction of nearly 100 ps from 0 to 5 kbar. The solid line is a

least squares fit to a phenomenological equation:

$$\tau = \tau_0 + \frac{\tau_s}{S + S_0} \quad (8.6)$$

The three phenomenological parameters from the fit are $\tau_0 = 171$ ps, $\tau_s = 98.3$ ps, and $S_0 = 0.98$ kbar. This model suggests a saturation value of 171 ps for large S . Although the agreement between this model and the experimental data is good, no efforts were made to investigate whether there are any Physical meanings to this equation.

In conclusion, non-exponential relaxation of photo-generated carriers was observed on n^+ -GaAs sample under $S \parallel [100]$ uniaxial stress by time resolved PL experiments. Stress dependence of various relaxation parameters p_0 , A , and B were studied at 100K. As the stress increases, we observed (a) an increase of p_0 , (b) a less yet observable increase of A , and (c) no appreciable change of B . The effective hole lifetime decreases with stress.

8.3.2 Exciton Relaxation in i -GaAs SQW/Si

In the bulk material, changes of the relaxation processes are due to the stress induced changes on the matrix elements as well as other electronic band structure parameters such as the effective masses. In semiconductor microstructures, other stress induced changes are also involved and may even become more important. In particular, the new electronic subbands formed by the new periodicity (or confinement) along the

z direction will be strongly altered by the application of the external uniaxial stress (see the preceding chapter). For example, as discussed in section 6.3.4, the LH-HH ordering of the valence bands in the GaAs QW/Si structures can be tuned by the stress. This stress tuning of the electronic subbands (and dispersion) is more dramatic than the bulk case and will significantly change the dynamic properties.

Shown in Fig. 76 are the PL spectra taken at 4K lattice temperature of an intrinsic GaAs SQW/Si under $S \parallel [100]$ for $S=0$ and 9.3 kbar. This is the same sample which has been characterized by the PR in section 6.3.4. The $S=0$ spectrum shows a dominant peak of 11L exciton at 1.500eV. The 11H exciton is observed as a high energy shoulder at 1.511eV. The low energy shoulder at 1.486eV is the $E_0(2)$ feature from the bulk GaAs buffer region. At $S=9.3$ kbar, the 11H feature becomes dominant at 1.513eV. The 11L feature now moves to the higher energy side due to external uniaxial stress and disappears. 11L energy shift has

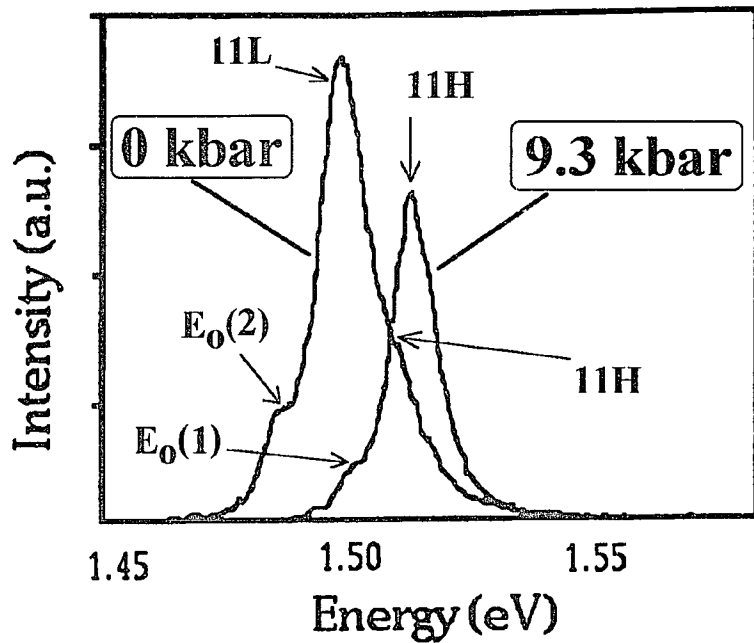


FIG. 76 PL spectra at 4K of a 200Å *i*-GaAs SQW/Si under $S \parallel [100]$ for $S=0$ and 9.3 kbar.

shoulder at 1.486eV is the $E_0(2)$ feature from the bulk GaAs buffer region. At $S=9.3$ kbar, the 11H feature becomes dominant at 1.513eV. The 11L feature now moves to the higher energy side due to external uniaxial stress and disappears. 11L energy shift has

been observed at intermediate stress magnitudes. The associated bulk GaAs edge $E_0(1)$ of 11H is observable at 1.501eV. The stress dependence of the transition energies agrees with the PR experiments discussed in the previous chapter.

Fig. 77 shows the PL time profile integrated between the high and low energy PL edges under 0 and 9.3 kbar. The thermalization and cooling of this system is mainly due to the lowest exciton subband. The cooling is through the relaxation of

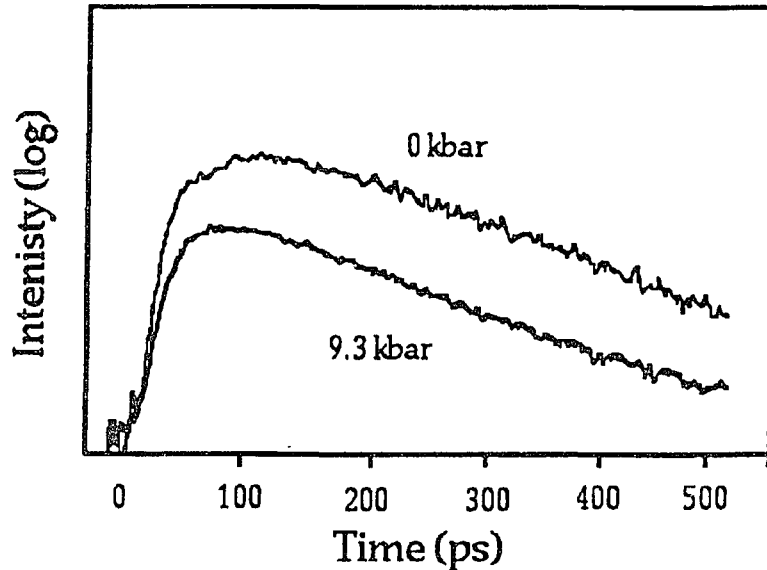


FIG. 77 Time dependent PL intensity profile for an *i*-GaAs SQW/Si under $S \parallel [100]$ for $S=0$ and 9.3 kbar.

the exciton center of mass motion (kinetic energy). At $S=0$, the 11L exciton shows slower rising time (0-120ps) than the 11H exciton at 9.3 kbar (0-80ps). The faster rising profile of 11H at 9.3 kbar may indicate the faster inter-subband relaxation process from the higher lying 11L subband to 11H subband. The exciton annihilation decay time is unchanged by the stress and estimated to be 170ps.

Average PL energy is used to determine the exciton energy relaxation process. The average PL energy is defined as:

$$\langle E(t) \rangle = \frac{\int_0^\infty dE I(E,t)E}{\int_0^\infty dE I(E,t)} \quad (8.7)$$

The experimentally obtained time dependent average energy $\langle E(t) \rangle$ is displayed in Fig. 78 for $S=0$ and $S=9.3$ kbar. The relaxation process is quite different from each other. At zero stress, the relaxation is nonexponential, which consists of a fast and a slow components. However, only a fast relaxation process is observed at 9.3 kbar.

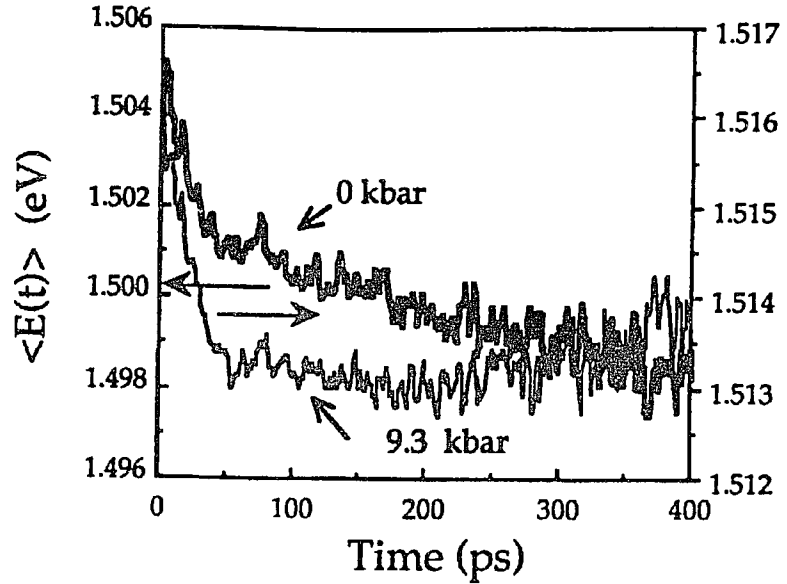


FIG. 78 Average energy $\langle E(t) \rangle$ relaxation of an *i*-GaAs SQW/Si under $S \parallel [100]$ for $S=0$ and 9.3 kbar.

We can determine the stress dependence of the various relaxation parameters by fitting the experimental $\langle E(t) \rangle$ curves to an exponential (single and double) decay model. The obtained relaxation time constants of both fast (open circles) and slow (solid circles) components are displayed in Fig. 79(a). The relaxation energy, defined as the energy difference of $\langle E(0) \rangle - \langle E(\infty) \rangle$ is also displayed in Fig. 79(b) as a function of

S. We see that the relaxation behavior changes a lot before and after the cross over point of the 11L and 11H transitions around 2-4 kbar. The fast relaxation component becomes faster when the ground state changes from 11L to 11H exciton, while the slow component has almost no change. After 3 kbar, the fast relaxation time constant becomes only about half of the value below 3 kbar. The fast component is due to exciton phonon interaction. When exciton effective mass changes from that of 11L to 11H

around 3 kbar, the exciton-LO phonon interaction may be affected.

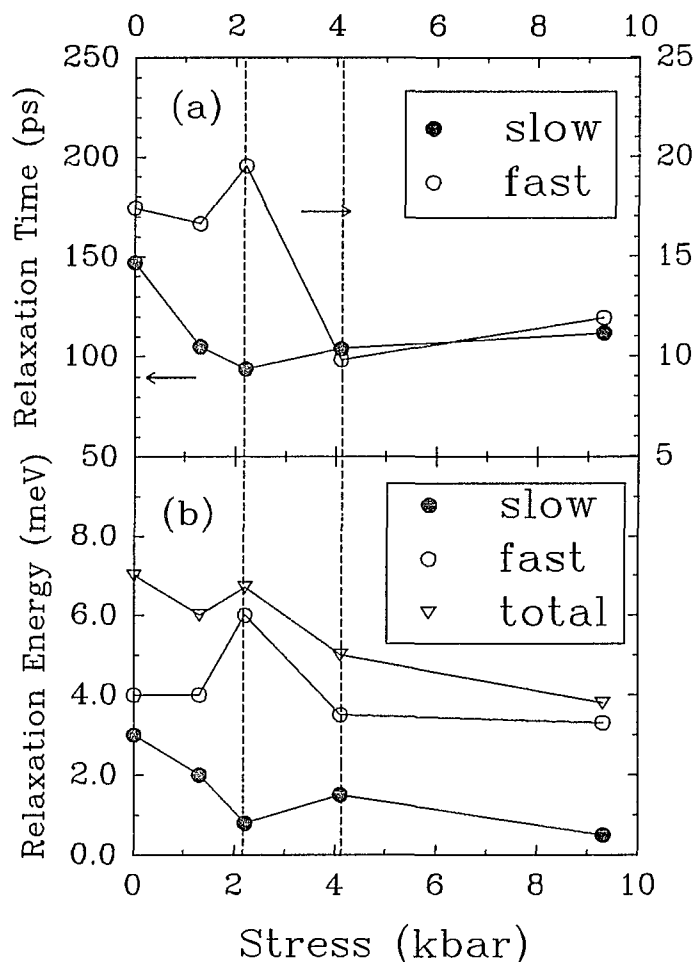


FIG. 79 Stress dependence of (a) relaxation time constants and (b) relaxation energies of both fast (open circles) and slow (solid circles) components in an *i*-GaAs SQW/Si structure.

8.3.3 Free Carrier Relaxation in p^+ -GaAs MQW/Si

The same experiment has also been carried out on a similar structure with initial doped holes. The 20 period 188Å/350Å GaAs/ $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ MQW structure was grown by MBE on (001) Si substrate with a 2μm GaAs buffer in between. The barrier

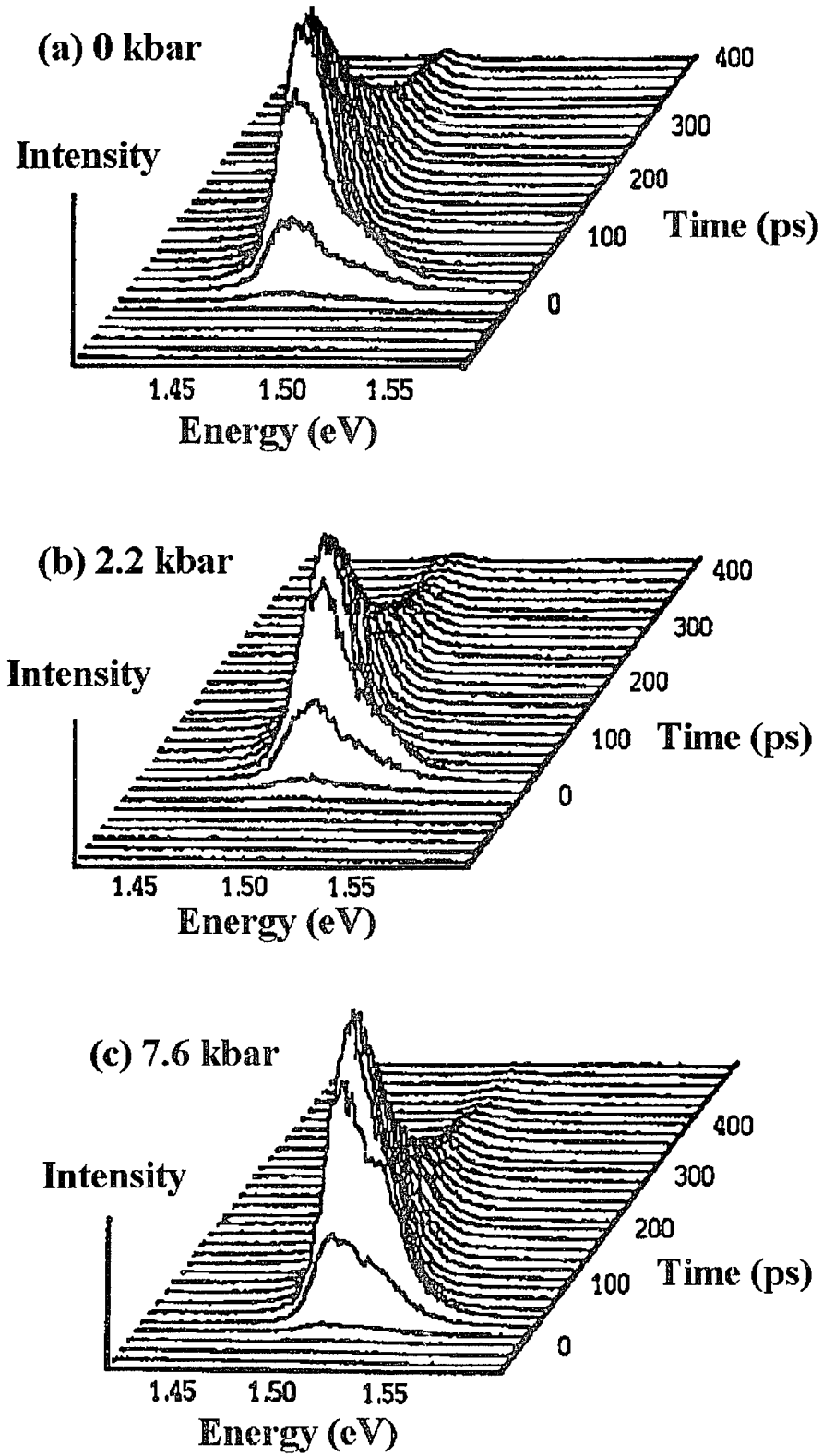


FIG. 80 Simultaneously energy and time resolved PL spectra at 4K of a 188Å p^+ -GaAs MQW/Si structure under $S \parallel [100]$ for (a) 0, (b) 2.2 kbar, and (c) 7.6 kbar.

thickness is 250Å in which a central region of 50Å is doped with Be atoms. The doping provides a hole density of $2.5 \times 10^{12} \text{cm}^{-2}$ in the wells with a Fermi energy of 12meV below the 11L subband edge at $S=0$. This is the system to study the free carrier dynamics instead of exciton behavior.

The simultaneously energy and time resolved PL spectra at 4K are shown in Fig. 80 for the sample under $S \parallel [100]$ with (a) 0, (b) 2.2 kbar, and (c) 7.6 kbar external in-plane uniaxial stress. The PL peak position shifts significantly to the high energy side from 0 to 2.2 kbar and then becomes relatively insensitive to the

stress (see 7.6 kbar spectrum). This is due to the cross over of 11L and 11H feature at 2kbar and different stress dependence of LH and HH features. The stress tuning of the band structure agrees with the PR and time resolved PL experiments on the 200Å *i*-GaAs SQW/Si structure. It also agrees with a theoretical calculation (squares) shown in Fig. 81, in which the band bending and the band gap renormalization effects due to the free carriers have been assumed to be stress independent and estimated from the 11L and 11H positions of PL spectrum at $S=0$.

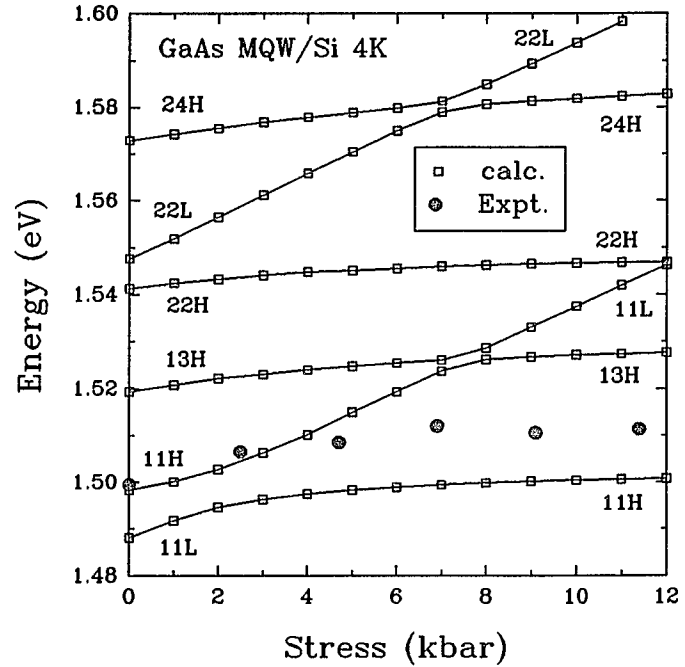


FIG. 81 Calculated transition energies of a 188Å p^+ -GaAs QW/Si structure at 4K.

Significant changes on the time profile can also be seen. For example, it is obvious that $S=7.6$ kbar spectrum shows faster relaxation process at the PL peak energy than the $S=0$ and 2.2 kbar spectra. This indicates that the different nature of the 11L ($S=0$ and 2.2 kbar) and 11H ($S=7.6$ kbar) ground states may play some role in the carrier dynamics changes.

Massive experimental data analysis is still in progress. One simple way is again to examine the relaxation of the average energy. The initial average energy $\langle E(0) \rangle$ at different stresses are plotted as solid circles in Fig. 81. Comparison with the calculation suggests that the major contribution to the PL signal always comes from the ground state subband, even if at $t=0$. Thus, the relaxation behavior of average energy should be dominated by the lowest conduction and highest valence subbands. The time dependent $\langle E(t) \rangle$ curves are shown in Fig. 82 for several different stresses. For $S < 7$ kbar, the $\langle E \rangle$ remains constant at initial 0-70 ps time range, and then starts to decay exponentially. For $S > 9$ kbar, the $\langle E \rangle$ increases from 0 to 70ps, then relaxes very fast between 70 and 100ps, and finally relaxes exponentially quantitatively similar to the $S < 0$ spectra.

Within $t < 70$ ps time range the dynamic process of $S > 9$ kbar spectra are quite different from the $S < 7$ kbar spectra. They show a distinctive slow turn on process. This may be due to a slow inter-subband carrier relaxation feeding channel. Using a simple coupled two subband model, which involves five levels, we can reproduce this

slow turn on phenomenon by assuming a inter-sub-band scattering time of 100 ps (Takiguchi *et al*, 1992). In another word, a 100ps scattering time from 2H to 1H subbands is suggested to explain the observed slow turn on of the carrier kinetic energies above 9 kbar, while only 30ps inter-subband scattering time of 1H-1L ($S < 2$ kbar) or 1L-1H ($2 < S < 7$ kbar) relaxation is expected to explain the absence of this phenomenon for the $S < 7$ kbar curves. This different inter-sub-band scattering rates is a

direct result of the altered valence subband structures due to large external uniaxial stress. For $S < 7$ kbar, the dominant scattering channel is either 1H-1L or 1L-1H

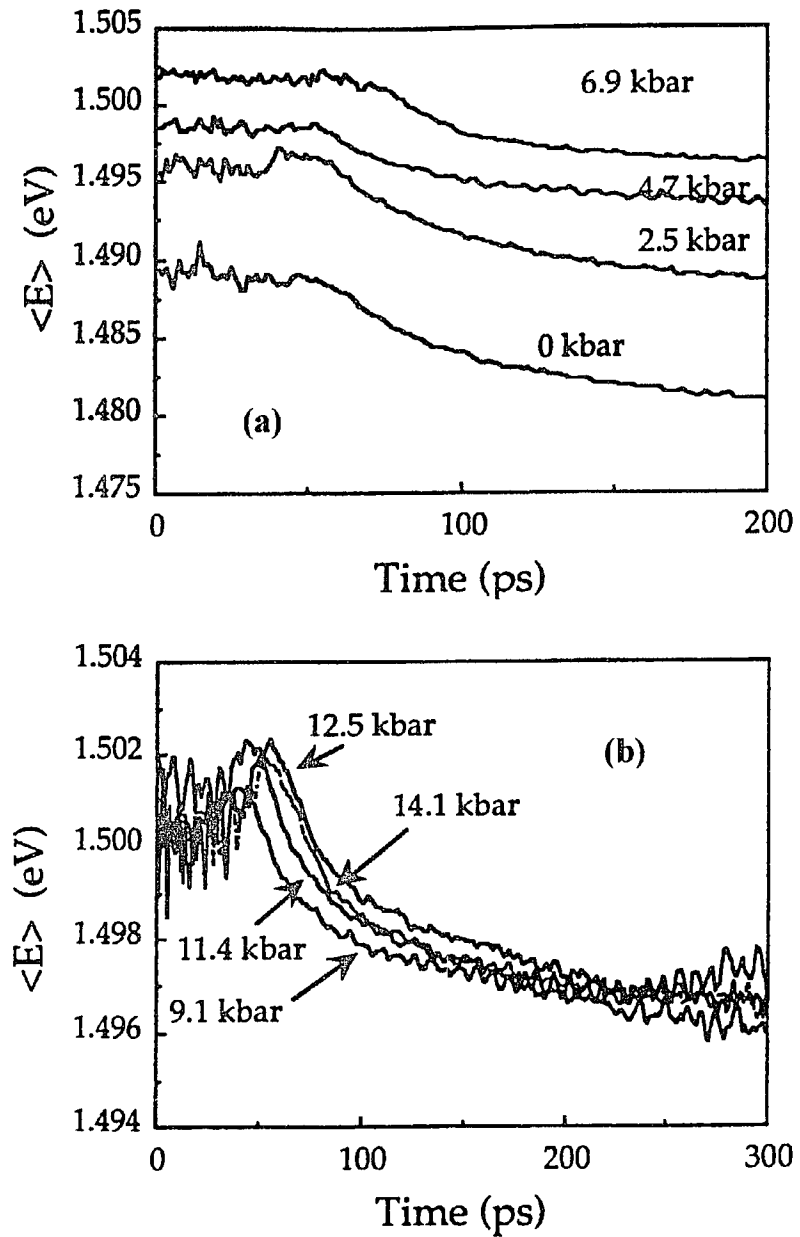


FIG. 82 Average PL energy relaxation of a p^+ -GaAs MQW/Si structure under $S \parallel [100]$ for (a) $S < 7$ kbar and (b) $S > 9$ kbar.

relaxations, while the 2H-1H relaxation takes over for $S > 9$ kbar (see Fig. 81). Due to the parity difference of envelope wavefunctions of these subbands, the overlap integral (which governs the inter-subband scattering rate) between the 2H and 1H levels are much smaller than the 1H and 1L pair. Therefore, for $S > 9$ kbar, the carriers obtain their kinetic energy slowly from the hot carriers in the higher lying levels in contrast to the $S < 7$ kbar situations.

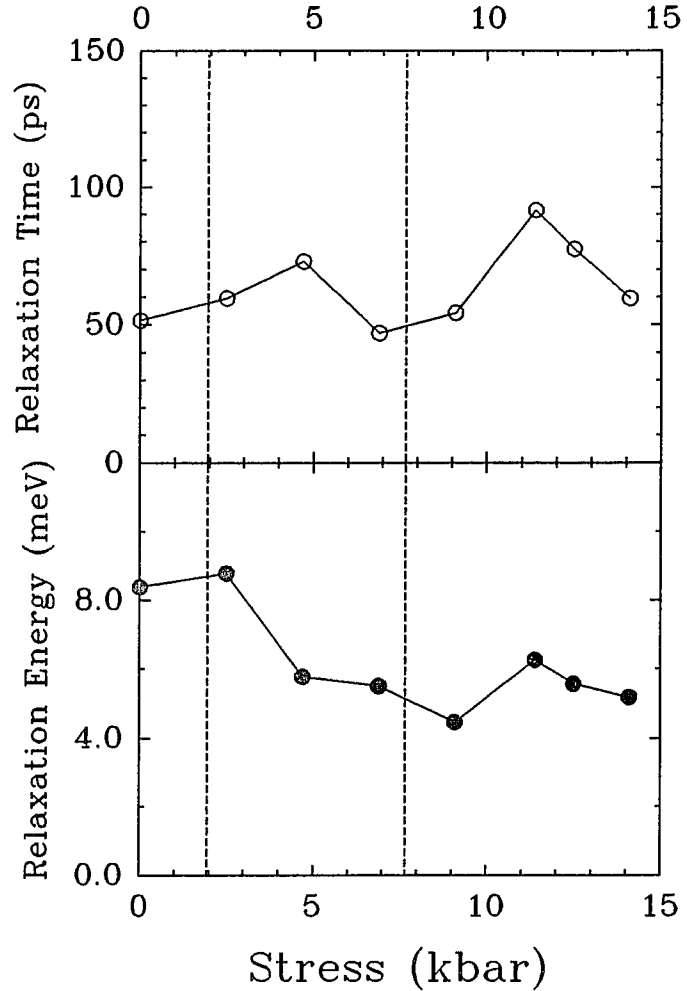


FIG. 83 Stress dependence of (a) relaxation time constants and (b) relaxation energies of both fast (open circles) and slow (solid circles) components in a p^+ -GaAs MQW/Si structure.

After initial 70-100ps, the kinetic energy relaxation is mostly due to the intra-subband cooling and electron hole recombination processes. The $S < 7$ kbar curves shows a single exponential decay while the $S > 9$ kbar curves are not single exponential. This difference can also be explained by the different inter-subband scattering time. We have used a single exponential decay constant model to estimate the effective relaxation time within this time region. The obtained stress dependent relaxation time constant as well

as the relaxation energy are plotted in Fig. 83. Changes around the 2 kbar and 8 kbar are observed, where the valence subband crossover occurs. When the stress increases, the relaxation time increases and the relaxation energy decreases. The relaxation energy difference may be due to the stress dependent photo-carrier generation efficiency.

8.4 Summary

- The influence of uniaxial stress on the carrier relaxation process was studied on a n^+ -GaAs bulk material. The relaxation parameters are affected by stress.
 - (a) A nonexponential decay was observed due to large carrier density. Three relaxation parameters, p_0 , A , and B , are extracted from experimental data.
 - (b) The initial photo-generated carrier density, p_0 , increases with stress, which is due to the effective mass change (band curvature change).
 - (c) The exponential relaxation component, A , increases slightly with stress due to the stress dependence of the dipole transition matrix element.
 - (d) The change of bimolecular recombination process parameter, B , is within our experimental error bar. The up limit of the stress dependence of this parameter is determined to be $< 2\% \text{ kbar}^{-1}$.
 - (e) An effective lifetime τ is proposed and found to decrease with stress which is modeled well by a phenomenological equation.
- Uniaxial stress influence on the exciton relaxation process in semiconductor microstructure is studied on an i^+ -GaAs SQW/Si sample where uniaxial stress is

used to tune the valence band structures, in particular, the HH or LH character of ground state.

- (a) PL energy domain confirms the exciton band structure changes tuned by the uniaxial stress.
 - (b) Average exciton kinetic energy relaxation is used to study the exciton dynamics. The relaxation consists of a fast and a slow components.
 - (c) The fast relaxation component due to exciton-LO phonon interaction depends on the exciton effective mass, which can be tuned by stress.
 - (d) The HH subband thermalization time is confirmed to be faster than the LH subband.
- Uniaxial stress influence on the carrier relaxation process in semiconductor microstructure is studied on p^+ -GaAs MQW/Si samples.
 - (a) Changes on the energy domain are consistent with the other studies.
 - (b) Average energy relaxation is used to study the carrier dynamics. The dynamic behavior for $S > 9$ kbar is dramatically different from the $S < 7$ kbar curves. For $S > 9$ kbar, we observed a slow turn on of the carrier kinetic energy at initial 0-70ps and then decays non-exponentially, while the opposite is true for $S < 7$ kbar.
 - (c) A simple five level model situation has been simulated. A inter-subband scattering time of about 100ps (30ps) is suggested for $S > 9$ kbar ($S < 7$ kbar) in order to reproduce the observed different behavior.

- (d) The relaxation time (relaxation energy) is found to increase (decrease) slightly with the external stress.

Chapter 9. Conclusions and Future Works

9.1 Conclusions

1. We show that modulation spectroscopy is a powerful tool.
2. Semiconductor microstructures show a lot of interesting properties which are different from bulk materials.
3. Various external perturbations can yield important information of the semiconductor microstructures and their influences are interesting in their own sense. The effects of temperature, electric field, and uniaxial stress are studied. Other perturbations such as magnetic field and hydrostatic pressure may as well be informative tools.
4. Several effects of various external perturbations studied in this work on semiconductor microstructures are:
 - Temperature:
 - (a) Temperature dependence of exciton line shape functions is studied.
 - (b) Quantum transitions are usually follow that of the well material.
 - (c) Broadening parameters show similar trend but quantitatively less dependent on the temperature in narrower wells.
 - (d) A linear relationship between Γ_{cp} and L_z is found which is attributed to the reduced Frohlich interaction in reduced dimensional systems.

- Electric field:
 - (a) QCSE in SQW.
 - (b) Larger Stark shifts of interwell transitions at low field and field tuning of coupling in CDQW.
 - (c) The role of electric field in HEMT structure is studied, which is essential to balance the Fermi level (doping) and result in significantly different intensities of various quantum transitions from that of the SQW at flat band condition.
- In-plane uniaxial stress:
 - (a) Effects are well described by deformation potential theory.
 - (b) LH/HH transitions have large/small stress dependence.
 - (c) LH transitions are not observed for $\mathbf{E} \parallel \mathbf{S}$ at high stress while HH transitions show up in all polarizations.
 - (d) Various effects due to piezoelectric field for the $\mathbf{S} \parallel [110]$ are observed.
 - (e) Different screening of piezoelectric field is observed between InGaAs/GaAs and GaAs/AlGaAs systems.
 - (f) In systems with built-in biaxial tensile stress a strong anticrossing with interesting polarization behavior is observed.
 - (g) Relaxation processes in n^+ -GaAs bulk and GaAs QW/Si structures are studied.

9.2 Future Works

1. Temperature effects

- The line shape functions of modulation spectroscopy need further studies.

- Further work is needed on the study of electron (exciton)-phonon interaction in reduced dimensional systems.
 - (a) Accumulate more experimental evidence, varying both L_z and systems.
 - (b) Large L_z SQW from 200Å to 1000Å (bulk).
 - (c) Smaller L_z SQW below 60Å, in order to (i) form an overall view of Γ_{cp} vs. L_z together with larger L_z results and (ii) possibly study the enhanced surface (interface) phonon effects.
 - (d) More detailed theory of electron (exciton)-phonon coupling in reduced dimensional systems such as the quantitative L_z dependence.
 - (e) Influences from other structure factors such as AlAs interface layers.
 - (f) Besides the 2D systems, study the 1D and 0D systems such as quantum wires and quantum dots, where this interaction will be dramatically changed since the dispersion curves (if exists) of both electron (exciton) and phonon are much more different in different dimensions.

2. electric field

- Study the phenomena arising from electric field influences on the various microstructures besides SQWs, e.g., SLs. For example, detailed line shape analysis could help us understand the Stark ladder formation in SLs as demonstrated in CDQW study.
- More work is needed on the study of HEMT structures.

3. uniaxial stress

- More systematic measurements on deformation potentials of various important bulk materials such as the compositional dependence of these values on ternary alloy materials. For example, linear interpolation between InAs and GaAs is the only approach used for InGaAs material although there are huge differences between two end materials (e.g. nearly twice on a). Also a parameter discontinuity is found on AlGaAs material. Further experimental and theoretical efforts are needed in order to understand its origin and universality.
- In-plane stress effects could be naturally extended to other semiconductor microstructures other than the QWs studied so far since the techniques and experiences are mature on thin wafer materials.
- Piezoelectric coupling may be a suitable tool in probing the surface/interface states density distribution.
- Various other methods besides the modulation spectroscopy and time resolved PL methods are yet to be used to study the various other property changes of semiconductor microstructures under high uniaxial stress.
- A growth directional uniaxial stress apparatus is currently under development. This will certainly be an aid in our systematic study in this area.

Appendix A. Publications

1. H. Qiang, Fred H. Pollak and Grayce Hickman, "Piezo-photorefectance of the direct gaps of GaAs and $\text{Ga}_{0.78}\text{Al}_{0.22}\text{As}$ ", Solid State Comm. 76, 1087-1091 (1990).
2. Y.S. Huang, H. Qiang, F.H. Pollak, G.D. Pettit, P.D. Kirchner, J.M. Woodall, H. Stragier and L.B. Sorensen, "Temperature dependence of the photorefectance of a strained layer $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ single quantum well", J. Appl. Phys. 70, 7537-7542 (1991).
3. Y.S. Huang, H. Qiang, F.H. Pollak, J. Lee, and B. Elman, "Electroreflectance study of a symmetrically coupled $\text{GaAs}/\text{Ga}_{0.77}\text{Al}_{0.23}\text{As}$ double quantum well system", J. Appl. Phys. 70, 3808-3814 (1991).
4. H. Qiang, F.H. Pollak, C. Mailhot, G.D. Pettit and J.M. Woodall, "Novel externally generated piezoelectric effect in semiconductor microstructures", Phys. Rev. B 44, 9126-9128 (1991). (Rapid Communication)
5. H. Qiang, F.H. Pollak, C. Mailhot, G.D. Pettit and J.M. Woodall, "Uniaxial stress study of the quantum transitions in a strained layer (001) $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ single quantum well", Preceedings of 5th International Conference on Modulated Semiconductor Structures, Nara, Japan (1991), and Surface Science 267, 103-106 (1992).
6. H. Qiang, F.H. Pollak, C. Sotomayor Torres, W. Leitch, M. A. Strosio, G.J. Iafrate, and K.W. Kim, "Size dependence of the electron-phonon coupling in $\text{GaAs}/\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ single quantum wells", Appl. Phys. Lett. 61, 1411-1413 (1992).
7. H. Qiang, F.H. Pollak, K. Shum, Y. Takiguchi, R.R. Alfano, S.F. Fang and H. Morkoc, "Piezospectroscopy of GaAs and $\text{GaAs}/\text{GaAlAs}$ single quantum wells grown on (001) Si substrates", Appl. Phys. Lett. 60, 2651-2653 (1992).
8. H. Qiang, Y.S. Huang, F.H. Pollak, G.D. Pettit, and J.M. Woodall, "Temperature dependence of the 11H photorefectance lineshape in an (001) $\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ single quantum well", Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE, Bellingham) 1678, 177-188 (1992).
9. S. Lee, K.M. Yoo, and R.R. Alfano, H. Qiang and F.H. Pollak, "Hole lifetimes in [001] uniaxial stressed GaAs", Phys. Rev. B. 47, 7036-7040 (1993).

10. Y. Yin, H. Qiang, F.H. Pollak, D. Streit, M. Wojtowicz, "Two dimensional electron gas effects in the electromodulation spectra of a pseudomorphic $\text{Ga}_{0.78}\text{Al}_{0.22}\text{As}/\text{In}_{0.21}\text{Ga}_{0.79}\text{As}/\text{GaAs}$ modulation-doped quantum well structure", *Appl. Phys. Lett.* **61**, 1579-1581 (1992).
11. K. Shum, Y. Takiguchi, J.M. Mohaidat, R.R. Alfano, H. Qiang, F.H. Pollak, and H. Morkoc, "Electron energy relaxation dynamics in GaAs quantum wells grown on Si: cool hole effect", *Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE, Bellingham)* **1677**, 249-260 (1992).
12. Y. Yin, H. Qiang, F.H. Pollak, D.C. Streit, and M. Wojtowicz, "Electromodulation spectroscopy of a pseudomorphic GaAlAs/InGaAs/GaAs modulation-doped quantum well structure: two-dimensional electron gas effects", *Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE, Bellingham)* **1675**, 498-510 (1992).
13. H. Qiang, F.H. Pollak, and R.N. Sacks, "Piezospectroscopy of a GaAs/GaAlAs single quantum well structure: piezoelectric effects", *Solid State Comm.* **84**, 51-55 (1992).
14. H. Qiang, F.H. Pollak, K. Shum, Y. Takiguchi, R.R. Alfano, S.F. Fang, H. Morkoc, "Effects of external uniaxial stress on GaAs microstructures grown on (001) Si substrates", presented at Electronic Materials Conference, MIT, Boston, June (1992).
15. F.H. Pollak and H. Qiang, "External and/or internal stress Effects on the optical properties of semiconductor microstructures", to be published in *Jap. J. Appl. Phys.*
16. Y. Yin, H. Qiang, D. Yan, F.H. Pollak, and T.F. Noble, "Room temperature photorefectance characterization of pseudomorphic GaAlAs/InGaAs/GaAs high electron mobility transistor structures including the two-dimensional electron gas density", to be published in *Semiconductor Sci. and Tech.*
17. Y. Takiguchi, K. Shum, R. Alfano, H. Qiang, F. H. Pollak, and H. Morkoc, "Picosecond electron thermalization in biaxially strained GaAs/AlGaAs quantum well grown on Si substrate under external uniaxial stress", presented at the IEEE LEOS Conference, Boston, Nov. (1992).
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19. H. Qiang, Y. Yin, D. Yan, F.H. Pollak, D. Huang, G. Gumbs, and T.F. Noble, "Optical detection of two dimensional electron gas features by modulation spectroscopy", presented at the International Conference on Luminescence and Optical Spectroscopy of Condensed Matter, Storrs, CT, (1993), and to be published in J. Luminescence.
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21. F.H. Pollak, H. Qiang, D. Yan, Y. Yin, and V. Boccio, "Better device yields with modulation spectroscopy", Photonics Spectra, 27, 78-84 (1993).
22. H. Qiang, E. Look, F.H. Pollak, K. Shum, Y. Takiguchi, R.R. Alfano, S. Fang, and H. Morkoc, "Photoreflectance study of GaAs/GaAlAs single quantum wells grown on (001) Si substrates", to be published in the Solar Energy Materials and Solar Cells.
23. G. Gumbs, D. Huang, Y. Yin, H. Qiang, D. Yan, and F.H. Pollak, "Many-body effects in the electromodulation spectra of modulation-doped quantum wells: theory and experiment", submitted to Phys. Rev. B.
24. H. Qiang, F.H. Pollak, K. Shum, Y. Takiguchi, R.R. Alfano, S.F. Fang, and H. Morkoc, "Effects of uniaxial stress on the optical properties of GaAs and GaAs/Ga_{0.7}Al_{0.3}As single quantum wells grown on (001) Si substrates", submitted to Phys. Rev. B.
25. H. Qiang, F.H. Pollak, Y.S. Tang, P.D. Wang, and C.M. Sotomayor Torres, "Characterization of process-induced strains in GaAs/Ga_{0.7}Al_{0.3}As quantum dots using room temperature photoreflectance", submitted to Appl. Phys. Lett.

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