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OPTICAL PROPERTIES OF GaAs/AlGaAs MULTIPLE QUANTUM WELLS GROWN IN THE [111] CRYSTALLOGRAPHIC DIRECTION(1)

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Photoreflectance measurements have been performed on high quality GaAs/AlGaAs multiple quantum wells grown along the [111] crystallographic direction. These measurements indicate that the heavy and light hole masses are 0.8 and 0.08, respectively, in the [111] direction of bulk GaAs. These values are in good agreement with the Luttinger parameters for GaAs. In addition, this investigation indicates that the band alignments of GaAs and AlGaAs are not very sensitive to crystallographic orientation.

Recent MBE growth studies [1] have shown that GaAs-AlGaAs multiple quantum wells (MQW) can be fabricated with the superlattice axis along a variety of crystallographic directions. This development has important implications in the study of the electronic and optical properties of MQW. Specifically, as a result of the anisotropy of the valence and conduction bands in bulk GaAs and the possible dependence of the AlGaAs/GaAs band alignment on crystallographic orientation, the band structures of these MQW are expected to differ. These differences are interesting because they allow the understanding of the relationship between the anisotropic bulk band structure of GaAs and that of the MQW to be probed. Furthermore, an understanding of this relationship is important technologically because it allows additional flexibility in the design of devices based upon particular features in the band structure of the MQW. In this paper, photoreflectance (PR) measurements [2] performed on [111]B MQW will be discussed. The results of this investigation are compared with interband optical studies on [100] MQW [3-5].

A series of MQW with well widths ranging between 90-400A have been grown by MBE on [111]B GaAs substrates. The 150K PR measurements were performed with a probe beam provided by a tungsten lamp and a 3/4 m spectrometer. The 5145A emission of an Ar ion laser served as the PR pump excitation. Fig. 1 shows the PR spectra obtained from three of the MQW. The lowest energy features in the PR spectra at 1.492 eV arise from excitonic transitions of the GaAs substrate, while the highest energy arrows correspond to excitonic transitions in the AlGaAs cap layers. A variety of other peaks are observed at energies between the GaAs and AlGaAs energy gaps. These features, whose number decreases as the width of the quantum wells is reduced, are assigned to excitonic transitions in the quantum wells. The labels in Fig. 1, nH(L), occur near the calculated energies of excitons associated with the energy gap between the n valence subband of heavy (light) hole character and n^{th} conduction subband. In this calculation, the energies of the k=0 subband states were determined from an effective mass square well model. The model included an energy-dependent effective electron mass to account for the conduction band nonparabolicity [6], and current conserving boundary conditions. The energy-dependence of the electron mass in the [111] direction was obtained from the 7 band k·p calculation of Rössler [7]. The energies of the nH(L) excitons are given by,

$$E_{nH(L)} = \varepsilon_{nH(L)} + \varepsilon_{nE} + E_{GaAs} - E_B(nH(L)), \qquad (1)$$

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where $E_B(nH(L))$ is the binding energy of the nH(L) exciton, E_{GaAs} is the energy gap of GaAs, and $\varepsilon_{nH(L)}$ and ε_{nE} are the n^{th} heavy (light) hole state and n^{th} electron subband state, respectively. In Eq. 1, we have employed exciton binding energies calculated for [100] MQW [8]. The exciton binding energies for [111] and [100] MQW are expected to be similar because the average in-plane heavy and light hole masses for [111] and [100] MQW do not differ greatly. In addition, we have assumed that the excitonic binding energy is not a function of subband index. The light and heavy hole masses, the relative band alignments of GaAs and AlGaAs and the quantum well width were treated as fitting parameters. Figure 2 shows a comparison between the observed and calculated excitonic energies for six {111} MQW. The peak positions of the excitonic transitions of the PR spectra were determined from the three point fitting procedure of Aspnes[9]. The excellent agreement between the model calculation and the experimentally determined excitonic transitions, evident in Fig. 2, was obtained with the values of the fitting parameters given in Table 1. A comparison between the magnitudes of the quantum well widths estimated from the growth conditions, L_g, and from the fit to the PR data , L_f, indicates that L_f is always ~5% smaller than that predicted from the growth parameters. This observation is consistent with the known characteristics of the MBE machine during the growth cycle. Specifically, the magnitude of L_g is expected to be accurate to within ±10%, but the reproducibility of the growth rate is expected to be better than ±2%. The heavy hole mass given in Table 1 for the [111] MQW is about 2.5 times larger than the value of 0.34 reported by Miller [3] for [100] MQW. In contrast, the light hole masses in the [100] and [111] MQW are similar at 0.09

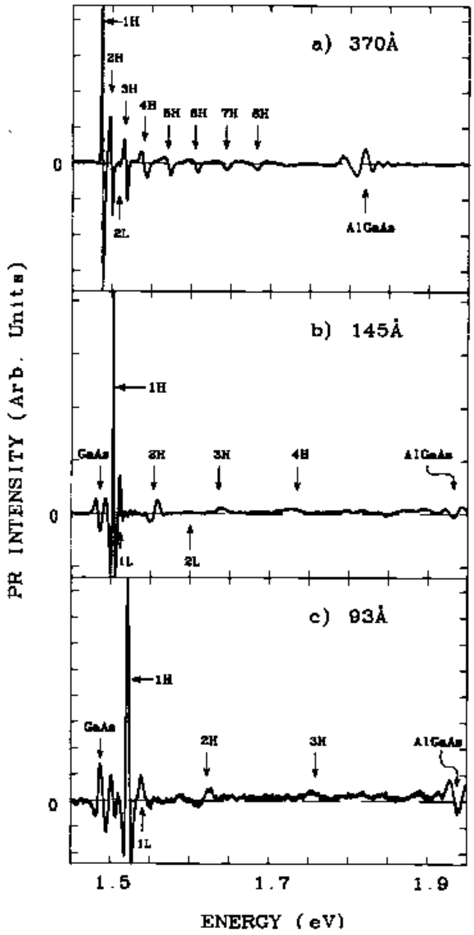


Fig. 1--150K PR spectra of [111] MQW with the indicated well widths. The nH(L) labels denote the energies of excitonic transitions predicted from a calculation employing the parameters given in Table 1.

Label	Sample	L_g (A)	L_f (A)	M_{hh}	M_{lh}	Q_e
a)	V899	100	93	0.8	0.08	0.55
b)	V898	150	145	0.8	0.08	0.55
c)	V897	200	198	0.8	0.08	0.55
d)	V896	250	238	0.8	0.08	0.55
e)	V894	300	287	0.8	0.08	0.55
f)	V895	400	370	0.8	0.08	0.55

Table 1--Summary of the magnitudes of the parameters employed in the model calculation. M_{hh} and M_{lh} label the heavy and light hole masses, L_g and L_f are the well widths estimated from the growth conditions and from the model calculation and Q_e is defined in Eq. 4.

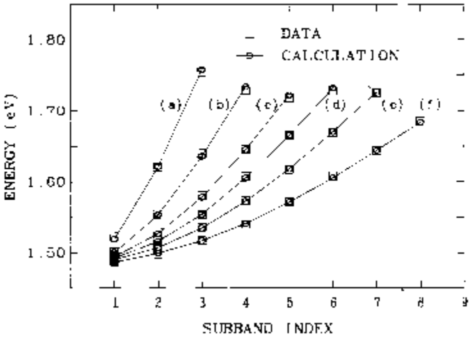


Fig. 2--A comparison between the observed and calculated excitonic energies in [111] MQW. The parameters employed in the fit are M_{hh}=0.8, M_{lh}=0.08 and Q_e=0.55. The well widths of curves (a)-(f) are given in Table 1. The lines serve as guides to the eye.

and 0.08, respectively. These observations illustrate the sensitivity of the optical properties of MQW to the growth direction.

The dispersion curves for the valence bands of GaAs as a function of the Luttinger parameters are given by,

$$(2) \qquad \varepsilon_{h,l} = -\tfrac{1}{2}\,\gamma_1 k^2 \pm [\gamma_2{}^2 k^4 + 3(\gamma_3{}^2 - \gamma_2{}^2)[k_x{}^2 k_z{}^2 + k_x{}^2 k_y{}^2 + k_y{}^2 k_z{}^2]]^{1/2},$$

where γ_1, γ_2 and γ_3 are the Luttinger parameters [10-12] and ε_h and ε_l are the energies of the heavy and light hole bands. The heavy and light hole masses, M_{hh} and M_{lh}, along the [100] and [111] directions are related to the Luttinger parameters through the following expressions:

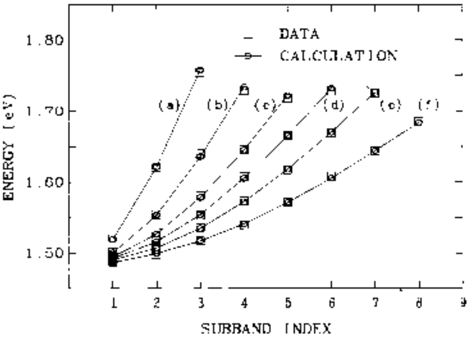
$$(3) \qquad \begin{array}{lll} M_{hh} = (\gamma_1 - 2\gamma_2)^{-1} & M_{lh} = (\gamma_1 + 2\gamma_2)^{-1}, & [100] \\ M_{hh} = (\gamma_1 - 2\gamma_3)^{-1} & M_{lh} = (\gamma_1 + 2\gamma_3)^{-1}. & [111] \end{array}$$

Table 2 presents a comparison of the masses arising from Luttinger parameters reported by others [10-12] for bulk GaAs and the masses that are required to fit the optical spectra from [100] and [111] MQW. This comparison indicates that the effective masses determined from the Luttinger parameters are in good agreement with the values determined from the optical studies of MQW and illustrates the sensitivity of the optical properties of MQW to the anisotropy of the bulk band structure. As a consequence of the uncertainties in quantum well width and excitonic binding energies for our samples, we are unable to determine which of the sets of Luttinger parameters given in Table 2 are in the best agreement with our measurments.

The relative band alignment of [100] GaAs-AlGaAs microstructures has been studied for a number of years and is commonly parameterized by [3],

$$(4) \qquad Q_e = \Delta E_c/(E_{AlGaAs} - E_{GaAs})$$

where ΔE_c is the conduction band offset and E_{AlGaAs} and E_{GaAs} are the energy gaps of AlGaAs and GaAs. Previous studies [3] of the band offsets on [100] MQW have yielded values of Q_e between 0.5-0.85. The most recent [4,5] (and assumed to be most accurate) values indicate that Q_e = 0.68. As can be seen from table 1, the PR measurements suggest that for the [111] MQW, Q_e = 0.55. Although this value is somewhat smaller than that for the [100] direction, the uncertainty in the magnitude of Q_e determined from the fit to the interband PR measurement only allows us to conclude that the band alignments of GaAs and AlGaAs are not much different in the [111] and



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$$\varepsilon_{h,l} = -\tfrac{1}{2}\gamma_1 k^2 \pm [\gamma_2^2 k^4 + 3(\gamma_3^2-\gamma_2^2)[k_x^2 k_z^2 + k_x^2 k_y^2 + k_y^2 k_z^2]]^{1/2}, \tag{2}$$

where γ_1, γ_2 and γ_3 are the Luttinger parameters [10-12] and ε_h and ε_l are the energies of the heavy and light hole bands. The heavy and light hole masses, M_{hh} and M_{lh}, along the [100] and [111] directions are related to the Luttinger parameters through the following expressions:

$$\begin{aligned} M_{hh} &= (\gamma_1 - 2\gamma_2)^{-1} \quad M_{lh} = (\gamma_1 + 2\gamma_2)^{-1}, \quad [100] \\ M_{hh} &= (\gamma_1 - 2\gamma_3)^{-1} \quad M_{lh} = (\gamma_1 + 2\gamma_3)^{-1}. \quad [111] \end{aligned} \tag{3}$$

Table 2 presents a comparison of the masses arising from Luttinger parameters reported by others [10-12] for bulk GaAs and the masses that are required to fit the optical spectra from [100] and [111] MQW. This comparison indicates that the effective masses determined from the Luttinger parameters are in good agreement with the values determined from the optical studies of MQW and illustrates the sensitivity of the optical properties of MQW to the anisotropy of the bulk band structure. As a consequence of the uncertainties in quantum well width and excitonic binding energies for our samples, we are unable to determine which of the sets of Luttinger parameters given in Table 2 are in the best agreement with our measurments.

The relative band alignment of [100] GaAs-AlGaAs microstructures has been studied for a number of years and is commonly parameterized by [3],

$$Q_e = \Delta E_c/(E_{AlGaAs} - E_{GaAs}) \tag{4}$$

where ΔE_c is the conduction band offset and E_{AlGaAs} and E_{GaAs} are the energy gaps of AlGaAs and GaAs. Previous studies [3] of the band offsets on [100] MQW have yielded values of Q_e between 0.5-0.85. The most recent [4,5] (and assumed to be most accurate) values indicate that $Q_e = 0.68$. As can be seen from table 1, the PR measurements suggest that for the [111] MQW, $Q_e = 0.55$. Although this value is somewhat smaller than that for the [100] direction, the uncertainty in the magnitude of Q_e determined from the fit to the interband PR measurement only allows us to conclude that the band alignments of GaAs and AlGaAs are not much different in the [111] and

				[100]		[111]	
Ref.	γ_1	γ_2	γ_3	M_{hh}	M_{lh}	M_{hh}	M_{lh}
a)	7.65	2.41	3.28	0.31	0.08	0.92	0.07
b)	6.85	2.10	2.90	0.38	0.09	0.95	0.08
c)	7.15	2.03	2.96	0.32	0.09	0.81	0.08
MQW	----	----	----	0.34	0.09	0.80	0.08

Table 2--The Luttinger parameters, γ_n, in Ref. a), b) and c) are obtained from references [10], [11] and [12], respectively. The heavy and light hole masses for [100] MQW are taken from reference 3.

[100] directions. This uncertainty does not arise from errors in determining the excitonic peak energies in the PR data or from the lack of agreement between the model and the experiment (which is quite good). Rather, it arises because we are unable to estimate the accuracy of incorporating an energy-dependent effective mass in our model. However, we note that if the energy-dependence of the electron mass is neglected or if the non-parabolicity characteristic of the [100] direction is employed in the model instead of that corresponding to the [111] direction, the agreement between the data and experiment is significantly poorer. Furthermore, under these circumstances the value of Q_e does not become larger than 0.65. Therefore, although our measurements indicate that the band alignments for [100] and [111] MQW are similar, additional studies, such as electronic Raman scattering [4], are necessary before a quantitative difference between the band alignments in the [111] and [100] directions can be stated with confidence.

In conclusion, we report PR measurements that explore the sensitivity of the optical properties of GaAs/AlGaAs MQW to the direction of the superlattice axis. The results of interband optical measurements of [111] and [100] MQW are in good agreement with the published values of the Luttinger parameters. Furthermore, as noted in previous studies [13], it appears that the relative band alignments of GaAs and AlGaAs are not very sensitive to the superlattice direction.

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