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FACTORS INFLUENCING ENERGY QUANTISATION

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ABSTRACT

Investigations of energy quantisation in a range of multiple quantum well (MQW) systems using effective mass band structure calculations including non-parabolicity in both the well and barrier layers are reported. Working with different values of band offsets and band gap differences, the results of the investigations show that energy quantisation is relatively more sensitive to band gap differences than to band offsets. For the particular case of the GaAs multiple quantum well systems, it is observed that while the 70:30 value of band offsets gave the best fit of theory to experiment for the electron-heavy hole transitions under parabolic band approximations, the electron-light hole transitions under the same parabolic band approximation support the 85:15 value. The inclusion of non-parabolicity however, supports values close to the 63:37 ratio. The factors observed to influence the confinement energies include the non consideration of the <n'0 transitions, lack of the exact knowledge of the heavy hole effective mass and the band gap difference in addition to the well-width.

KEY WORDS: Energy quantization, effective mass, band structure, non-parabolicity, band offsets, band gap.

INTRODUCTION

The controversy over the values of the band-offsets, a parameter which happens to be very essential for the evaluation of quantum well, has opened the experimentalist to the task of having to decide on which among the range, of available values to be used when attempting to fit his experimental observations to theoretical data. Ironically, that the very well studied of the Superlattices (SL) and Multiple Quantum Well (MQW) systems, the GaAs/AlGaAs system has witnessed a great deal of controversy is unfortunate.

The suggestion *(Miller et al, 1984a,b)* for the revision of the initial value of 85:15 < Eg for the band-offsets parameter given by *Dingle et al, (1974)* to 57:43 <Eg *(Miller et al, 1984a,b)* came ten years after the "Dingle, rule" was established. The investigations which resulted in this suggestion were carried out on parabolically shaped quantum wells. Though the use of the parabolic structure was noted to have increased the sensitivity of the confinement energy to the band offsets, the lack of control of the aluminum flux during growth has been pointed out by *Duggan (1985)* to imply that a parabolic potential has to be synthesized by systemic and precise adjustment of alloy and binary widths during deposition. Dawson et al (1985, 1986) and Duggan et al (1985) have carried out frontline investigations in the above regard.

This paper reports on the investigations carried out on a range of GaAs/$Al_xGa_{1-x}As$ MQW (x = 0.3) using the traditional optical absorption (OA) and photoluminescence (PL) measurements and an effective mass band structure calculations including non-parabolicity in both the well (GaAs) and the barrier ($Al_xGa_{1-x}As$) layers *(Adelabu, 1993, 1995, 1998)* to ascertain those factors that influence energy quantisation. The very near attempt to the present study is that on GaInAs/AlInAs MQW system by *Welch et al (1984)* which adopted the single quantum well model and pointed out that the inclusion of non-parabolicity in the barrier layer would lower the values obtained in their calculations.

THEORETICAL CONSIDERATION AND CALCULATION

In the work reported here, we have in a similar manner to *Bastard (1981) and Adelabu et al (1988, 1989) and Adelabu (1993, 1995, 1996, 1998)* used the dispersion relation:

$$CosQD = Cosk_1d_1\ Cosk_2d_2 - \tfrac{1}{2}(z+1/z)\ sink_1d_1 sink_2d_2. \quad \ldots\ldots\ldots\ldots(1)$$

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Table 1: Values of parameters used in calculations

Parameter	Material	
	GaAs	$Al_xGa_{1-x}As$
Energy gap*	Eqn(4) eV	$E_g(T) + 1.27x(eV)$
Electron mass**	$0.067m^*_o$	$(0.067 + 0.083)m_o$
Heavy hole mass**	$0.45m_o$	$(0.45 + 0.2)m_o$
Light hole mass**	$0.082m_o$	$(0.082 + 0.068)m_o$

* Casey and Panish 1978

** Jiang 1984

(x is the aluminum mole fraction while m_o is the free electron mass).

The same expressions with the appropriate parameters were used for the calculations of the confinement energies for the three charge carriers (electron, heavy hole and light hole) just in line with earlier work *(Adelabu, 1993, 1995, 1998)*.

where

$$k_1 = (2m^*_1E/\hbar^2)^{1/2}$$

$$k_2 = \{2m^*_2(E-V_o)/\hbar^2\}^{1/2}$$

and $$z = \frac{m^*_1k_2}{m^*_2k_1}$$

V_o is the barrier height, E is the energy eigenvalue and m^*_1, m^*_2 are the given respective effective masses. The subscript 1 refers to GaAs while 2 refers to $Al_xGa_{1-x}As$. Non-parabolicity was included *(Adelabu et al, 1988, 1989 and Adelabu, 1993, 1995, 1996, 1998)* in both the well and the barrier via:

$$\hbar^2k^2_1 = 2m^*_{o1}(E + X_iE^2) \text{ for the well} \quad .....(2a)$$

and

$$\hbar^2k^2_2 = 2m^*_{02}(E - V_o) + \kappa_2 (E - V_o)^2] \text{ for the barrier} \quad ..... (2b)$$

where κ_i are the appropriate non-parabolicity constants, m^*_{oi} are the appropriate band-edge effective masses while all other parameters have their meanings as earlier given. The non-parabolicity constant a_1, were calculated using

$$\kappa_i = \frac{(1-m^*_1/m_o)^2}{E_g(T)} \quad .....(3)$$

where $E_g(T)$ is the appropriate band gap for the particular material at various temperatures. The energy gaps at various temperatures between 0-300K were calculated for GaAs, the well material using the expression as reported in *Adelabu (1993)*, viz:

$$E_g(T) = 1.519 - 5.405 \times 10T^2/(204 + T) \quad .....(4)$$

while those for $Al_xGa_{1-x}As$ were calculated using the expressions in Table 1.

EXPERIMENTAL METHODS

The MQW wafers used in the investigations, which were obtained from Essex University in Britain, were grown by Molecular Beam Epitaxy (MBE) on <100> semi-insulating GaAs substrate.They consisted of 100 unintentionally doped well (nominal well-width ranging from 4.6nm to 11nm) and 99 unintentionally doped $Al_xGa_{1-x}As$ barriers (nominal barrier-width of 10nm).

The specimens for the absorption spectra measurements were prepared *(Adelabu et al, 1997, 1998)* by selectively etching the substrate through a "two-stages" etching processes of fast etching (H_2SO_4:H_2O_2:H_2O, 1:8:1 by volume) and slow etching (H_2O_2 buffered to a pH of 7.05 with dilute ammonium hydroxide). The specimens for the PL measurements on the other hand required no special treatment but ordinary cleaning with acetone.

For the OA measurements, which were carried out between 12K and room temperature, the specimens were mounted over a hole in a copper heatsink attached to a variable cryostat with a drop of varnish at diagonal corners. The tungsten filament lamp of a UNICAM 700C-spectrophotometer was employed as the illumination source while the spectra measurements were detected using a PbS

detector with the incident light being perpendicular the MQW layers.

The PL spectra measurements were carried out between 9K and room temperature also using a variable temperature cryostat. The 647nm line of a CW-Krypton laser was used as the excitation source. The beam was focused on the sample defining a spot of radius of the order of 300μm. Orthodox lock-in-techniques, in conjunction with 1/3m monochromator and a cooled GaAs photomultiplier were used to disperse and detect the luminescence. The resolution in the measurement range of 1.40 eV and 1.80 eV was better than 0.5 meV. Temperatures were monitored in both cases with iron-doped gold versus chromel thermocouple located near the samples.

RESULTS AND DISCUSSIONS

Fig. 1 shows typical transmission/absorption spectra at room temperature of specimens with well-widths of (a) 11.0nm (b) 8.0nm (c) 4.6nm. Fig. 2. shows typical PL spectra of the 4.6nm well specimen at the low temperatures of 8K and 61K.

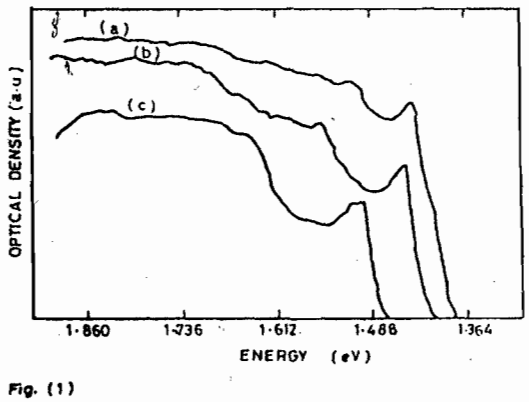

Fig. (1)

Fig. 1 Typical transmission/absorption spectra of a 100 period, 10.0nm barrier $GaAs/Al_{0.3}Ga_{0.7}As$ MQW structures at room temperature

a. Nominal well width of 11.0nm
b. Nominal well width of 8.0nm
c. Nominal well width of 4.6nm

For the interpretations of the spectra, the peak structures were translated as excitonic *(Dingle et al, 1974)* while their energy positions at the various temperatures were extracted. These were subsequently compared with the theoretical data as done by *Adelabu (1993, 1995,)*. Considering only the transition at the gamma valley (i.e., K = O), different band-offset values have been used in calculations at various temperatures. Here, an assumption is made that only the energy gap but not the confinement energy varies with the temperature.

Figs. (3)-(6) present some of the results of the

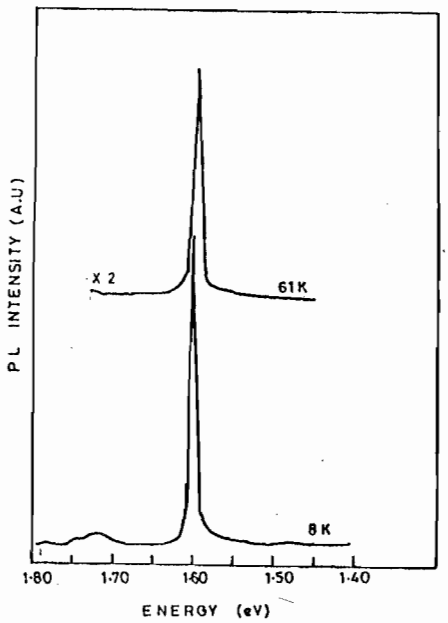

Fig. 2 Typical photoluminescence spectra for a 100 period, 10.0nm barrier, 4.6nm well $GaAs/Al_{0.3}Ga_{0.7}As$ MQW structures at 8K and 61K. The spectra are arbitrarily vertical displaced for clarity.

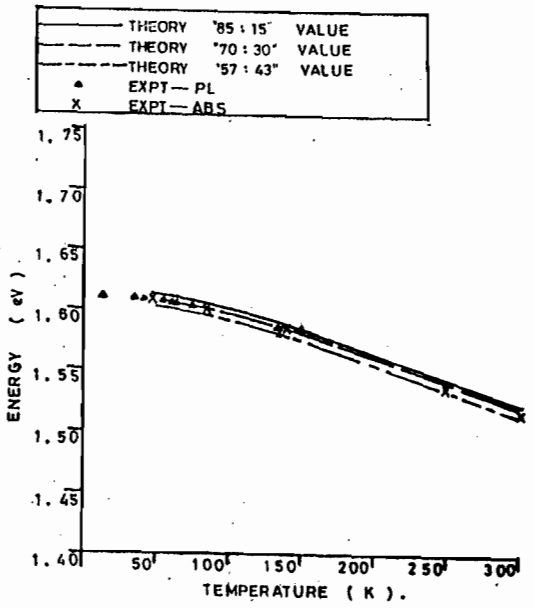

Fig. 3 Comparison of experimental 1E-1HH transitions with theoretical data assuming a parabolic band approximation at the band offset values of 85:15, 70:30 and 57: 43.

(<) Experimental points for photoluminescence (x) Experimental points for absorption measurements. The value of band gap difference used in calculation is 374 meV (Casey and Panish 1978)

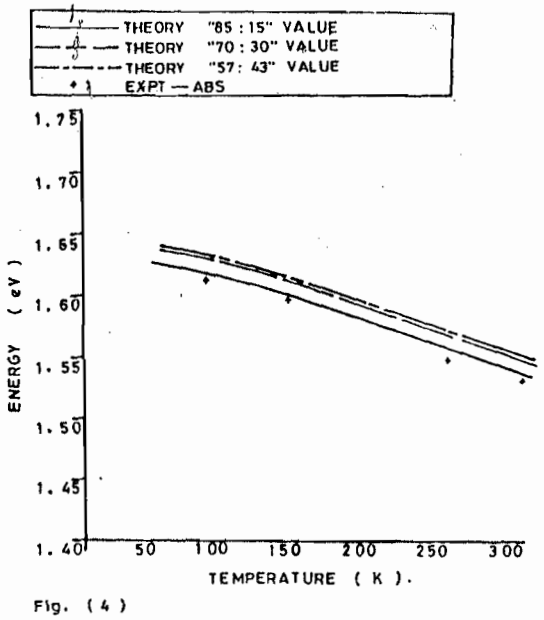

Fig. 4 Comparison of experimental 1E-1HH transitions with theoretical data assuming a parabolic band approximation at the band offset value of 85:15, 70:30 and 57:43. The value of band gap difference used in calculation is 374 meV (Casey and Panish, 1978), (+) experimental points for absorption measurements.

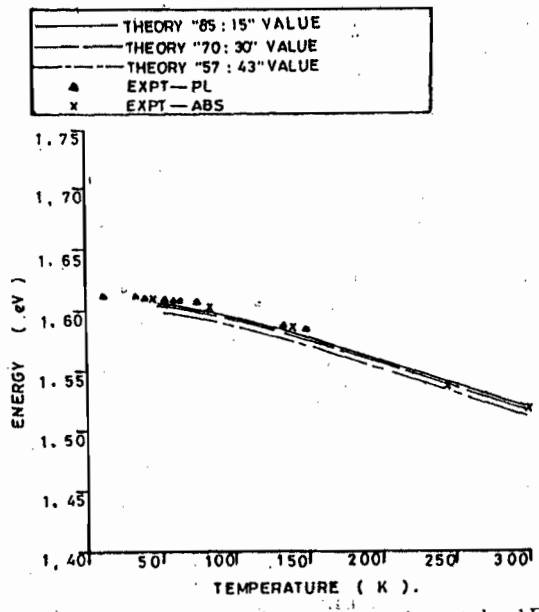

Fig. 5 Comparison of experimental 1E-1HH transitions with theoretical data, including nonparabolic in both the well and in the barrier material at the band offset values of 85:15, 70:30 and 57:43 and $<E_g$ = 374meV (Casey and Panish, 1978).

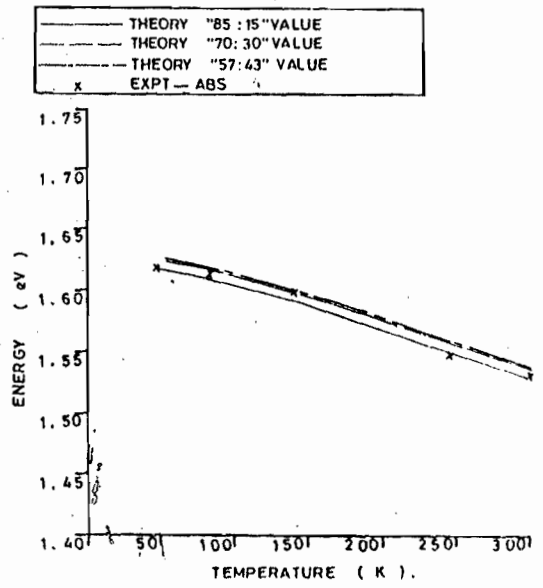

Fig. 6 Comparison of experimental 1E-1LH transitions with theoretical data, including nonparabolic in both the well and in the barrier material at the band offset values of 85:15, 70:30 and 57:43 and $<E_g$ = 374meV (Casey and Panish, 1978).

comparison of experiment with theory for the particular sample with the well-width of 4.6nm on which both the electron heavy hole (E-HH) and the electron light hole E-LH) transitions were experimentally observed in the investigations. The results of this sample is presented because its well-width falls within the range where the confinement energies are expected to be extremely sensitive to the band offsets parameter. In computing these figures, the band offsets of 85:15 $<E_g'$ 70:30 $<E_g$ and 57:43 $<E_g$ (conduction band: valence band) were used.These values were chosen because they are the largest, middle and least values reported in the literature *(Dingle et al, 1974, Dingle, 1975, Miller et al, 1984a,b, Dawson et al 1985, 1986, Duggan et al, 1985,*

The theoretical calculations only gave the sub-band transitions and not the exciton transitions that are experimentally observed. Thus, the exciton binding energy *(Jiang 1984)* has been added to the observed experimental transition energy. These values were used because the binding energies dependence on well-width and on the alloy compositions were taken into consideration in obtaining them.

For the E-HH transitions under parabolic band approximation (fig. 3) the 70:30 $<E_g$ values

gave the best fit of theory to experiment. On the other hand, the consideration of the E-LH transitions under the same approximation (fig. 4) opposes such a conclusion but rather supports the 85:15 $<E_g$ value. A careful observation of the curves in figs. 3 and 4 shows that there is the positioning of the curves. This observation is justified on the following ground. From the calculation of the confinement energies, it is observed that while these energies increase with the increase in band offsets in the case of the electron (i.e., the conduction band), they decrease with an increase in band offsets in the case of both the heavy hole and light hole (i.e., valence, band). The variation is greater in the case of the light hole than in both the electrons and heavy holes. This makes E-LH transition to be higher in energy for the 57:43 $<E_g$ value of the band offsets than the 85:15 $<E_g$ value (as shown in fig. 4). When non-parabolicity is included as described in equations (2) and (3) using the relevant parameters as given in Table 1, the results as presented in fig. (3) and (6) *(Adelabu, 1993)* for the E-HH and E-LH transitions respectively, support the about 70:30 $<E_g$ value if the average numerical deviations are considered. Some of the possible explanations are given below.

In the work by *Duggan (1985)*, it has been pointed out that the sensitivity to the band offset ratio is increased only by studing MQW and SL with narrow wells, transitions where $<ng0$ or by altering the well shape to be parabolic for instance. Duggan (1985) has pointed out the adverse effect of the latter. While it is agreed that the confinement energies may be very sensitive to band offsets for narrow wells of less than 3.0nm, however, the 4.6 nm well sample is sufficiently thin enough to produce about the same sensitivity as would be expected for less than 3.0nm. Moreso, it is worthy to think of the effect of the unavoidable topological disorder at the very thin wells which might introduce a significant adverse effect on the well width and consequently on the confinement energies *(Weisbuch et al, 1981)*.

Based on a careful fitting of the $<n=0$ (allow transitions), it has been observed that results can lead to the conclusion that the valence band offset lies in the range 0.3-0.4. Theoretical calculations of the (1E-3HH) transitions at two different aluminum mole fractions (x) for five different well widths and three different band offsets values are presented in Table 2. The result show that these transitions

Table 2: 1E-3HH Transition ($<=2$)

Band Offsets	Well Widths (nm)				
	4.6	5.0	5.5	6.0	6.5
85:15					
ΔE_g	NT	NT	NT	NT	NT
x = 0.3	NT	NT	NT	NT	NT
x – 0.35					
70:30	NT	NT	170:883	158:727	145:462
ΔE_g	NT	NT	185:269	168:487	152:076
x = 0.3					
x = 0.35					
	NT	209:260	190:930	171:965	154:281
60:40	NT	225:806	202:040	180:053	161:038
ΔE_g					
x = 0.3					
x = 0.35					

*NT implies no 3HH energy level within the well and consequently no 1E-3HH transitions should be expected. The values tabulated are 1E+3HH confinement energies.

are not present at all for the two mole fractions at the three bands offsets for a 4.6nm well sample. This is because the 3HH level, as revealed by the model calculations, is out of the well in all these cases. In addition, Table 2 reveals that the same things exist for the 5.0nm sample for the 85:15 $<E_g$ and 70:30 $<E_g$ values of the band offsets. Furthermore, the 85:15 $<E_g$ values reveal that these transitions are not possible for the 5.5nm, 6.0nm and 6.5nm well samples. These observations are consistent with the results of *Dawson et al (1985)* presented in their fig. 4, where the E_{3h} contours corresponding to the energies of the observed transitions seemed to have terminated around this range of well widths.

Another point is the lack of exact knowledge of the heavy hole effective mass *(Miller et al, 1984a,b)*. The values of the heavy hole effective mass used in the calculations, which happened to be more prominent in the literature are given in Table 1. Calculations were made using other values. These revealed differences ranging from 0.6meV to 3.82meV among the various values of the heavy hole effective masses reported in the literature. The values proposed by *Miller et al (1983a,b)* have not been used because they are much more smaller than the other reported values. The odds against this set of values have been exhaustively discussed by *Duggan (1985)*.

The dependence of the confinement energies on the band gap differences *(Adelabu and Abdullahi, 1997)* assuming that $Al_xGa_{1-x}As$ has a direct energy gap for Al mole fraction x with value of $x<0.45$ and that it obeys the relation:

$$E_g(0<x<0.45) = 1.247x$$

(Batey et al, 1985) for the gamma valley, is shown in fig. 7. When compared with the dependence of confinement energies on band offsets (fig. 8), the results reveal that the confinement energies are more sensitive to band gap difference than to band offsets.

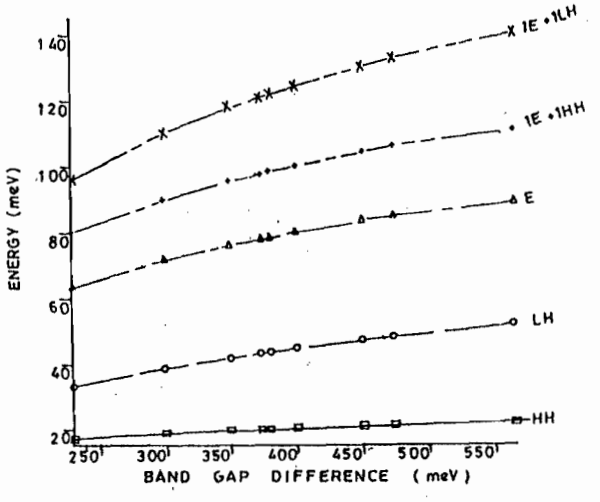

Fig. 7. Variation of confinement energies with the band gap difference for a 4.6nm well sample in GaAs/AlGaAs MQW at 70:30 band offset value.

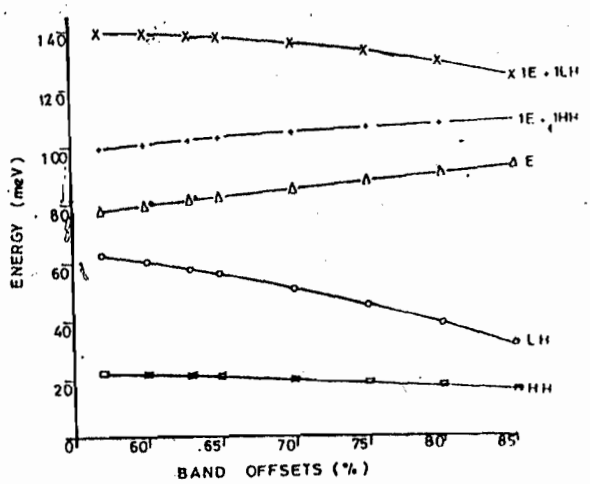

Fig. 8. Variation of confinement energies with the band offset values for a 4.6nm well sample in GaAs/AlGaAs MQW at $<E_g$ = 374meV (Casey and Panish, 1978) band gap difference.

CONCLUSION

Based on the results of the investigations presented here, it is concluded that to make a more meaningful decision on the value of the band offsets, it is very necessary to consider together the E-HH and the E-LH transitions employing both the parabolic and non-parabolic band approximations. The results indicate that the confinement energies are relatively more sensitive to band gap difference than to band offsets.

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