ON THE BAND GAPS AND BAND OFFSETS OF TYPE I MULTIPLE QUANTUM WELL (MQW) SYSTEM

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ABSTRACT

This work aims at investigating the comparison between experiment via optical absorption (OA) and photoluminescence (PL) and theory via envelope function approximation model vis-à-vis the band gaps and band offsets of type I multiple quantum well (MQW) system.

Measurements of optical absorption (OA) and photoluminescence (PL) have been carried out on type I Multiple Quantum Well (MQW) system of GaAs-AlGaAs grown by molecular beam epitaxy (MBE). An attempt has been made to compare exciton peak obtained for both heavy hole and light hole at band offset of 70/30 at different temperatures (Theory and Experiment). It is revealed from our investigation that the confinement energies of the particles increase with increase in the height of the potential barrier for electron and decrease with increase in height of the potential barrier for light hole and heavy hole. The increase is more pronounced in the case of the light hole.

However, our findings revealed clearly that the confinement energies of the particles vary as the band offsets.

Keywords: *Bandgap, Band Offsets, Multiple Quantum Well, Optical Absorption, Photoluminescence, Molecular Beam Epitaxy.*

1. INTRODUCTION

The band-gap in between valence and conduction bands is of key interest for all semi-conducting properties. Infact, many of the interesting properties of Multiple Quantum Well (MQW) structures are determined quantitatively by (i) difference in the band gap ΔE_g of the two components forming the MQW system as shown in figure I, and the band offsets ΔE_c and ΔE_v (which is the fractional distribution of the band gap difference between the conduction band and the valence well established in the case of GaAs-AlGaAs, the quantities, ΔE_c and ΔE_v have witnessed a great deal of controversy with values ranging 57% and 85% for the former and 43% and 15% for the latter. Nevertheless, ΔE_g for a given aluminium composition exhibits a range of values in the literature and thus even this quantity cannot be assumed to be beyond disput. For example, [1] have reported that the energy gap of $Al_xGa_{xz}As$ is a given function of x. This will consequently lead to varying ΔE_g, even for the same value of x, there will still be some uncertainties in the ΔE_g since the control of the shutter cannot be exact.

The most direct approach to the problem has been via optical techniques, notably via measurement of optical absorption [2, 3] among others and luminescence [4, 5, 6, 7, 8, 9]. The early work of Dingle and co-workers [2] gave the value of the parameter as 85/15 while the lowest figure of 57/43 was obtained by [7] using parabolically shaped quantum wells. Many other studies, among which are those by [10, 11, 4, 8] tend to favour a figure near the arithmetic mean of 70/30 for the $\Delta E_c/\Delta E_v$.

Another variable is the theoretical model used to interprete the optical data [11], Early interpretations [2, 3,] and a host of other literature were based on the particle-in-a box model. This is now superceded by such models as the envelop function model [12], the K.P model [13, 14] or the tight-binding model [15]; [16, 17] which takes into account light and heavy hole mixing. While valence band effects may be quite complex, they do not have a large effect on optical absorption and luminescence. Hence, a straight forward envelop function model applied to electrons, light hole and heavy holes may be regarded as adequate to interprete optical spectra, provided non-parabolicity is included [11].

It is the mission of this paper to present the results of investigations of optical absorption and luminescence spectra measurements and their interpretations using the envelop function model including non-parabolicity with particular reference to GaAs-AlGaAs grown by molecular beam epitaxy.

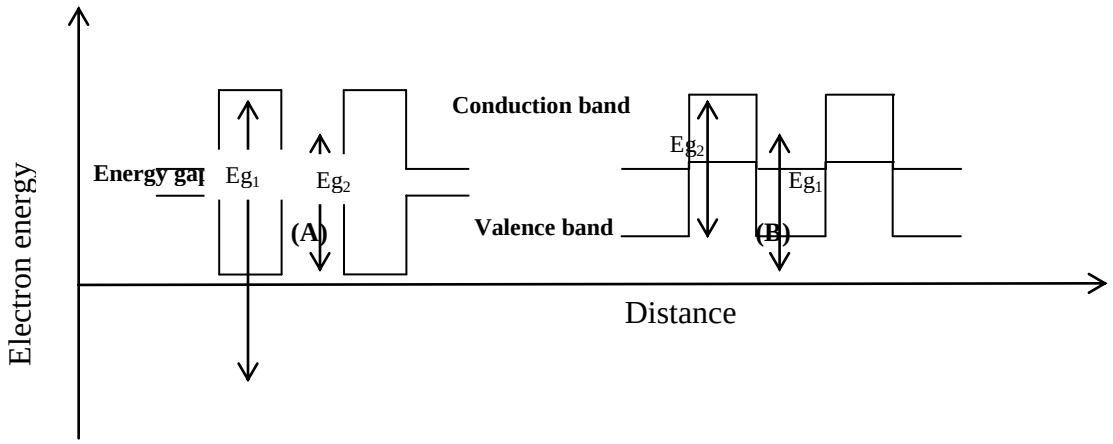

Figure 1: Periodic Potential for (A) type 1 MQW and (B) type II MQW

Experimental Measurements

The samples used which were obtained from Essex University, Britain, were grown by molecular beam epitaxy on a <100> InP substrate .Both optical absorption (OA) and photolumescence (PL) spectra measurements were carried out. They consisted of GaAs/$Al_{0.}Ga_{0.2}$As multiple quantum well.

The well-widths of the samples ranged between 50Å to 110Å, while the barrier width was fixed at 100Å, each sample had a period of 100. All the specimens for optical absorption were prepared by first mechanically polishing the substrate and then followed by chemical etching (which is the removal by chemical means of the substrate at the spot of illumination). While the luminescence spectra measurements were made with the 647nm line of a CW-Krypton laser absorptions spectra measurements were made with a UNICAM 700C spectrophometer. Temperatures were assumed with an iron-doped gold versus Chronel thermometer (with a reading error of ± 0.05k) located near the specimensat the tip of a variable temperature cryostat.

Theoretical consideration and Calculations

The theoretical calculations adopted for the interpretations of the experimental results are similar to those in [11, 18]; [19, 20]. In the calculations, the super lattice (SL) and (MQW) wave functions are taken as linear combination of plane waves inside layers of each components materials (i.e GaAs and AlGaAs), while the usual effective mass boundary conditions at two successive SL and MQW interfaces [12]; [21] were applied making use of Bloch's theorem. These led to the dispersion relation

$$CosQD = Cosk_1 d_1 Cosk_2 d_2 - \tfrac{1}{2}(z + 1/z) Sink_1 d_1 Sink_2 d_2 \quad \text{(i)}$$

Where $D = d_1 + d_2$ is the periodicity length, Q and K_1 are the wavelength components. d_1 and d_2 are the layer thicknesses of material 1 (AlGaAs) and material 2 (GaAs), and $z = m_2 * k_1 / m_1 * k_2$

Non-parabolicity is included via the relation between the wave vector and the energy as follows [11]

$\hbar^2 k_1^2 / 2m^*_{01} = (E - V_O)[1 + \alpha_1 (E - V_O)]$ (ii)

$\hbar^2 k_2^2 / 2m^*_{02} = E(1 + \alpha_2 E)$ (iii)

$m^*_1 / m^*_2 = [1 + 2\alpha_1 (E - V_O))] / (1 + 2\alpha_2 E)$ (iv)

Where V is the barrier height or well-depth, m^*_{01} is the band edge effective mass, α_i is the non-parabolicity constant (i=1,2) and E is the energy eigenvalue. The subscript 1 refers to the barrier (AlGaAs) while 2 refers to the well (GaAs).

2. RESULTS AND DISCUSSIONS

Typical absorption spectra of our specimens are shown in fig. 2 while fig. 3 presents typical photoluminescence spectra. As usual [11] the peak structures are translated as excitonic transitions between sub-bands [2, 3]. Before applying the model (as contained in equation i and ii), it is necessary to take into account the excitonic bonding energy and the effect of strain resulting from the absorption measurements. The strain effect was evident from the observed discrepancies between the absorption moles, the luminescence peaks and is associated with the chemical etching of the substrate at the spot of illumination. The values of the excitonic bonding energies which were

subtracted from the energy eigen values derived numerically from equation (i and ii), were taken to be those of [22]. These values took into account the necessary variation as a function of well-width and mass discontinuity. We have assumed that the energy shift between the luminescence peak (which is higher) and the absorption peak observed for the lowest energy transition, which was 13meV on the average, was applicable to all transition. Thus we have made corrections accordingly to all our absorption data.

The results of our calculations of the particle states at different band offsets are given in table Table 1.0 presents the variation of eigen values HH, LH, E, the transistion (IE+IHH) and the trasistion (2E+2H). The results in the table clearly revealed that for any particular band offset, the eigen value increase as the well width decreases. Also, it shows that while the electron confinement energy, transition eigen values for (IE + HH) and (2E + 2HH) decrease down the table, both the confinement energies for HH and LH increase down the table with a tremendous increase in the case of LH. The observation is due to the fact that as the conduction band or the potential barrier height for the electron decreases that for the hole increases in other to keep the band gap difference for the particular MQW system constant. Thus it is observed that the confinement energies of the particles increase with the height of the potential barrier. The increase is more pronounced in the case of light hole.

Figure 4.0 present the energetic position of the HH and LH excitonic peak (theory and experiment) at band offsets of 70/30. A close look at the fittings of experimental data to theoretical data as presented in figure 4 reveals that there is very good agreement. This is confirmed with the aid of computer using one way analysis of variance (ANOVA) and revealed that there is no significant difference between theory and experiment.

Table 1.0: Confinement energy for electrons, heavy holes, and light holes in the sample with well width of 10nm and 5nm at different band edge discontinuities.

Band Edge Discontinuity	5nm HH	10nm HH	5nm LH	10nm LH	5nm E	10nm E	5nm 1E+1HH	10nm 1E+1HH	5nm 2E+1HH	10nm 2E+1HH
85/15	14.1289	5.2506	29.7852	8.1236	84.3915	38.4583	98.5203	43.7089	319.2368	175.0836
80/20	15.6563	5.6006	36.6597	11.2314	81.973	37.677	97.6293	37.677	310.9631	133.3971
75/25	16.7064	5.7279	42.4821	12.1124	80.191	31.5036	96.8974	37.2315	302.1484	131.265
65/35	18.4885	6.0143	51.4559	13.0344	75.2904	30.6126	93.7789	36.6269	282.4189	126.8099
60/40	19.0931	6.1098	55.2427	14.1225	72.5537	29.7852	91.6468	35.895	271.5039	124.1051
57/43	19.428	6.2936	57.1894	16.3624	70.7465	29.387	90.7745	35.6806	265.0456	122.3905

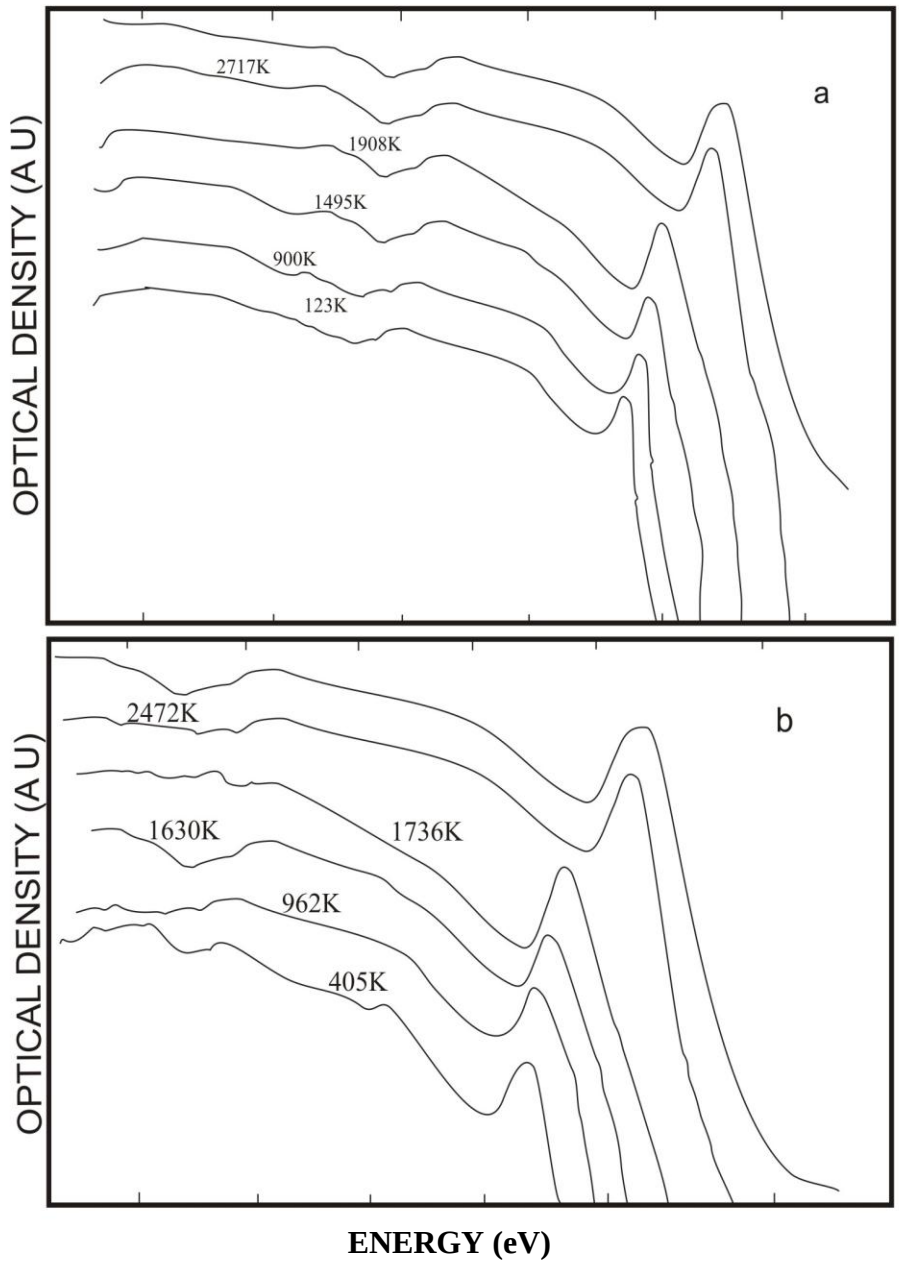

Figure 3: Typical absorption spectra of samples with well-width of a = 10nm, b=5nm

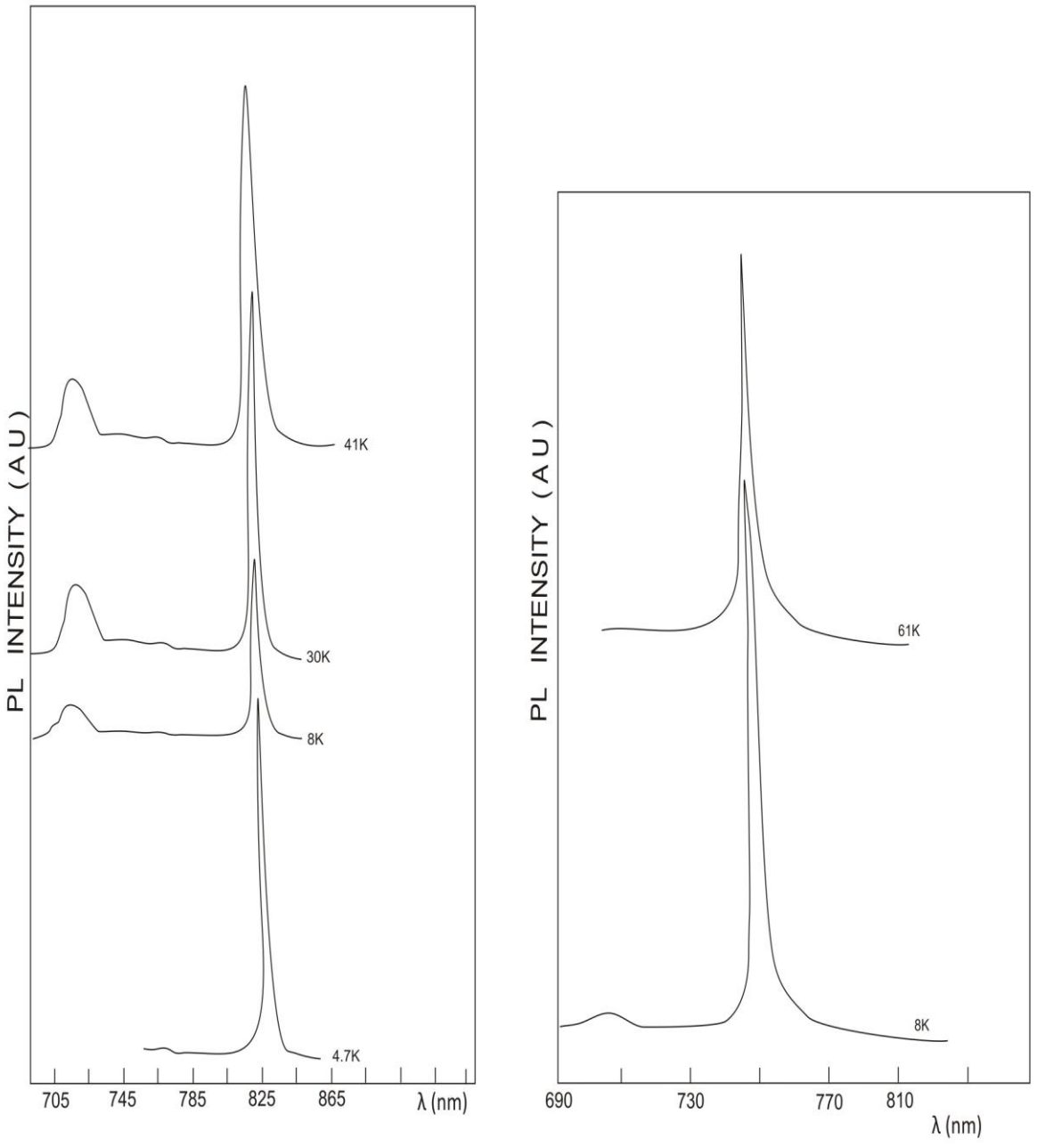

Figure 2: Typical photoluminescience spectra of sample with well-width of a=10nm, b=5nm

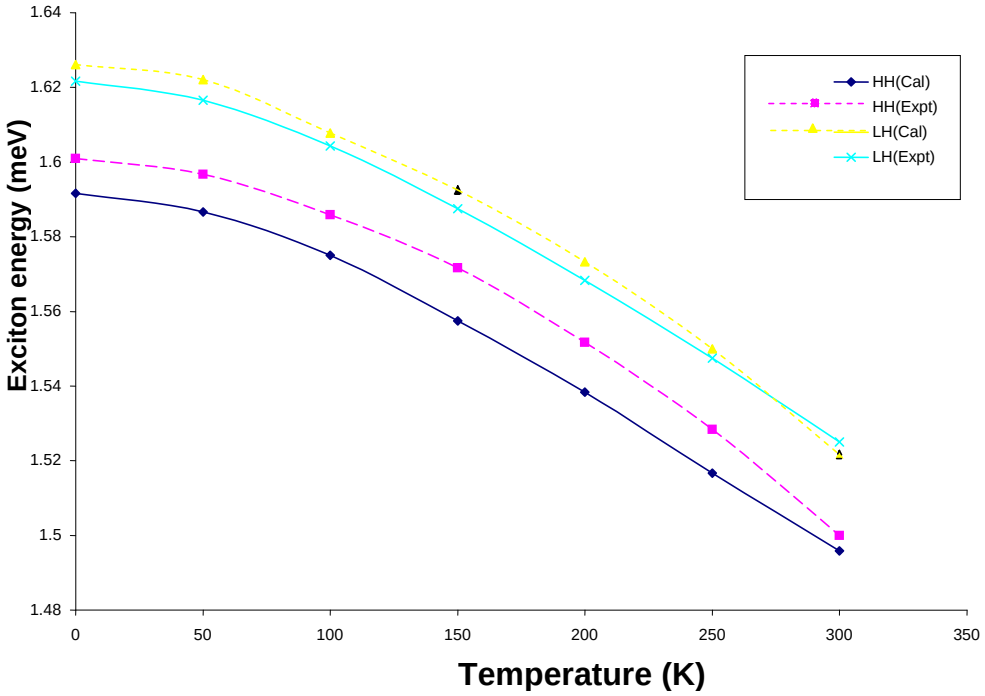

Figure 4.0: Comparison of Heavy hole and light hole exciton peak at ratio $\Delta E_c/\Delta E_v$ (70/30) at different temperatures for GaAs/AlGaAs heterostructure

3. CONCLUSION

We have carried out measurement of (OA) and PL on type I MQW system of GaAs/AlGaAs grown by molecular beam epitaxy. The comparison of experimental result with the calculated result shows a close agreement of the two. Calculation actually mimic experiment as evident in figure 4. It is revealed from our investigation that confinement energies of the particles vary as band offsets.

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