

On the Band Gaps and Band Offsets of Type I Multiple Quantum Well (MQW) System

J.S.A. Adelabu, J.O. Ajayi and A.O. Awodugba
Department of Physics, University of Abuja, FCT, Abuja, Nigeria

Abstract: 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 the 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.

Key words: Optical absorption, photoluminescence, exciton peak, confinement, potential barrier

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 difference in the band gap ΔE_g of the two components forming the MQW system as shown in Fig. 1 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, Casey and Panish (1978) have reported that the energy gap of $Al_xGa_{1-x}As$ 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 (Dingle *et al.*, 1974; Dingle, 1975) and luminescence (Dawson *et al.*, 1985; Miller *et al.*, 1980, 1981, 1984; Rogers and Nicholas, 1985; Weisbuch *et al.*, 1981). The early research of Dingle *et al.* (1974) gave the value of the parameter as 85/15 while the lowest figure of 57/43 was obtained by Miller *et al.* (1984) using parabolically shaped quantum wells. Many other studies, among which are those by Adelabu and

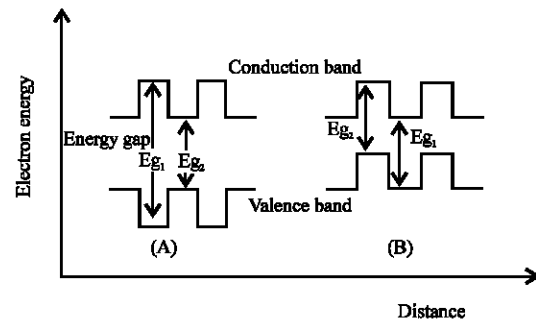


Fig. 1: Periodic Potential for (A) type I MQW and (B) type II MQW

Abdullahi (1987), Dawson *et al.* (1985) and Rogers and Nicholas (1985) 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 interpret the optical data (Adelabu, 1993), early interpretations (Dingle *et al.*, 1974; Dingle, 1975 and a host of other literature) were based on the particle in a box model. This is now superseded by such models as the envelop function model (Bastard, 1981), the K.P. Model (Bastard, 1982; Bastard *et al.*, 1984) or the tight-binding model (Schulman and McGill, 1979), (Schulman and Chang, 1983, 1985) 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 interpret optical spectra, provided non-parabolicity is included.

It is the mission of this research to present the results of investigations of optical absorption and luminescence spectra measurements and their interpretations using the envelop function model including non-parabolicity.

MATERIALS AND METHODS

Experimental measurements: Both Optical Absorption (OA) and Photoluminescence (PL) spectra measurements were carried out. The specimens used in the investigations were grown by Molecular Bean Epitaxy (MBE). They consisted of GaAs/Al_{0.2}Ga_{0.8}As MQW. The well-widths of the samples ranged between 50-110Å 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 647 nm line of a CW-Krypton laser absorptions spectra measurements were made with a UNICAM 700C spectrophotometer. Temperatures were assumed with an iron-doped gold versus Chronel thermometer (with a reading error of ±0.05k) located near the specimens at 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 by Adelabu (1993, 1999) and Adelabu *et al.* (1988, 1989). 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 (Bastard, 1981; White and Sham, 1981) were applied making use of Bloch's theorem. These led to the dispersion relation:

$$\text{Cos}QD = \text{Cos}k_1d_1\text{Cos}k_2d_2 - \frac{1}{2}\left(z + \frac{1}{z}\right)\text{Sin}k_1d_1\text{Sin}k_2d_2 \quad (1)$$

Where:

- D = d₁+d₂ = The periodicity length
- Q and K₁ = The wavelength components
- d₁ and d₂ = The layer thicknesses of material (AlGaAs) and material 2(GaAs)

RESULTS AND DISCUSSION

Typical absorption spectra of the specimens are shown in Fig. 1 while Fig. 2 presents typical

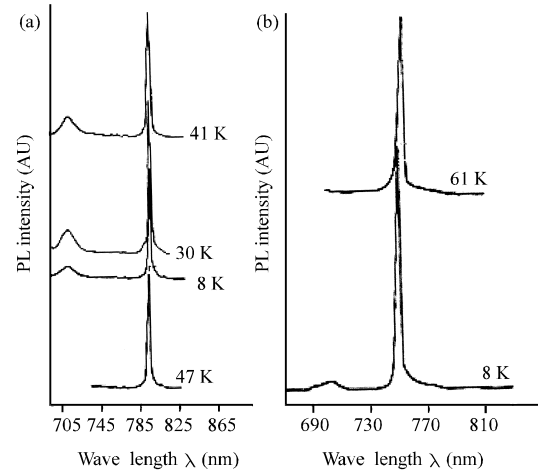


Fig. 2: Typical photoluminescence spectra of samples with well-width of a = 10 nm, b = 5 nm

photoluminescence spectra. As usual (Adelabu, 1993) the peak structures are translated as excitonic transitions between sub-bands (Dingle *et al.*, 1974; Dingle, 1975). Before applying the model (as contained in Eq. 1 and 2), 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 Eq. 1 and 2 were taken to be those of Jiang (1984). These values took into account the necessary variation as a function of well-width and mass discontinuity. Researchers 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 13 meV on the average was applicable to all transition. Thus, researchers have made corrections accordingly to all the absorption data. The results of the calculations of the particle states at different bond offsets are given in Table 1.

Table 1 presents the variation of eigen values HH, LH, E, the transition (1E+1HH) and the transition (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 (1E + 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

Table 1: Confinement energy for electrons, heavy holes and light holes in the sample with well width of 10 and 5 nm at different band edge discontinuities

Band edge discontinuity	5 nm (HH)	10 nm (HH)	5 nm (LH)	10 nm (LH)	5 nm (E)	10 nm (E)	5 nm (1E+1HH)	10 nm (1E+1HH)	5 nm (2E+1HH)	10 nm (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	81.9730	37.6770	97.6293	37.6770	310.9631	133.3971
75/25	16.7064	5.7279	42.4821	12.1124	80.1910	31.5036	96.8974	37.2315	302.1484	131.2650
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	35.8950	271.5039	124.1051
57/43	19.4280	6.2936	57.1894	16.3624	70.7465	29.3870	90.7745	35.6806	265.0456	122.3905

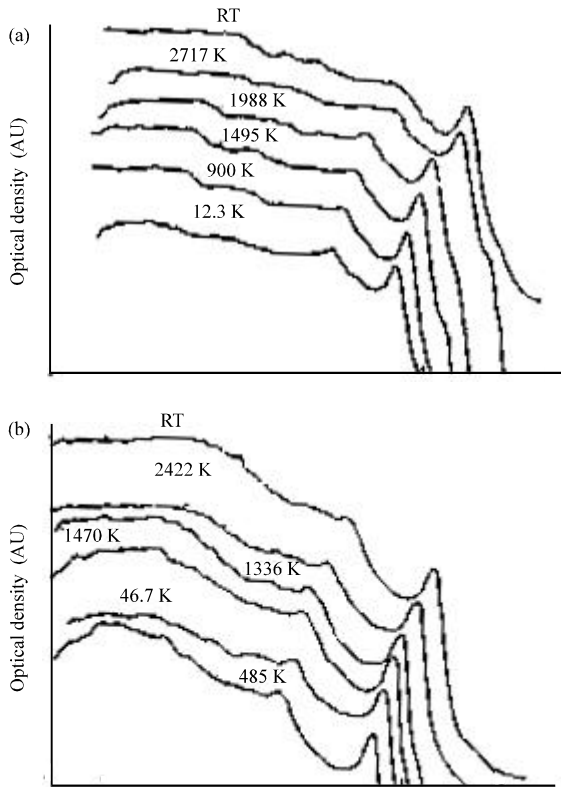


Fig. 3: Typical absorption spectra of samples with well-width of a = 10 nm, b = 5 nm

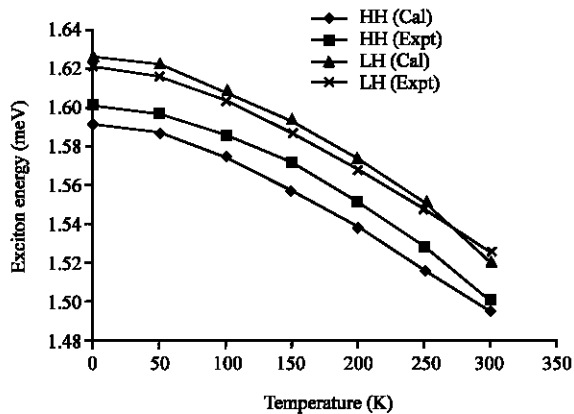


Fig. 4: Comparison of heavy hole and light hole exciton peak at ratio $\Delta E_c/\Delta E_v$ (70/30) at different temperatures for GaAs/AlGaAs heterostructure

that for the hole increases in order 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 (Fig. 3).

Figure 4 presents 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 Fig. 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.

CONCLUSION

Researchers 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 mimics experiment as evident in Fig. 2 and 3. It is revealed from the investigation that confinement energies of the particles vary as band offsets.

REFERENCES

Adelabu, J.S.A. and G.L. Abdullahi, 1987. Measurement of band-gap difference in GaAs MQW systems. *Global J. Pure and Appl. Sci.*, 3: 109-117.

Adelabu, J.S.A., 1993. On the interpretation of optical spectra in GaAs/AlGaAs SL and MQW systems. *Physica B.*, 183: 264-270.

Adelabu, J.S.A., 1999. Quantum confinement in synthetic solid state semiconductors. *J. Pure and Appl. Sci.*, 2: 47-52.

Adelabu, J.S.A., B.K. Ridley and G.J. Davies, 1989. Room temperature optical absorption and confinement effect in GaInAs/AlInAs MQW. *Semicond. Sci. Technol.*, 4: 677-681.

Adelabu, J.S.A., B.K. Ridley, E.G. Scott and G.J. Davies, 1988. Energy levels and optical absorption associated with GaInAs/AlInAs MQW. *Semicond. Sci. Technol.*, 3: 873-878.

- Bastard, G., 1981. Superlattice band structure in the envelope function approximation. *Phys. Rev.*, B24: 5693-5697.
- Bastard, G., 1982. Theoretical investigations of superlattice band structure in the envelope function approximation. *Phys. Rev.*, B25: 7584-7597.
- Bastard, G., O.U. Ziemelis, C. Delalande, M.I. Voos, A.C. Gossard and W. Wiegmann, 1984. Bound and Virtual bound states in semiconductor quantum wells. *Solid State Commun.*, 49: 671-674.
- Casey, H.C. and M.B. Panish, 1978. *Heterostructure Lasers, Part A: Fundamental Principles*. Academic Press, New York, pages: 189.
- Dawson, P.L., G. Duggan, H.J. Ralph, K. Woodbridge and G.W.T. Hoof, 1985. Positions of the sub-band minima in GaAs-AlGaAs quantum-well heterostructures. *J. Superlattices and Microstructures*, 1: 231-235.
- Dingle, R., 1975. Confined carrier quantum states in ultra thin semiconductor heterostructures. *Festkörperprobleme, Adv. Solid State Phys.*, 15: 21-48.
- Dingle, R., W. Wiegmann and C.H. Henry, 1974. Quantum states of confined carrier in very thin AlGaAs-GaAs heterostructures. *Phys. Lett.*, 33: 827-830.
- Jiang, T.F., 1984. An alternative approach to exciton binding energy in GaAs/AlGaAs quantum wells. *Solid State Commun.*, 50: 589-593.
- Miller, R.C., A.C. Gossard, W.T. Tsang and O. Munteanu, 1982. Extrinsic Photoluminescence from GaAs quantum wells. *Phys. Rev.*, B25: 3871-3877.
- Miller, R.C., D.A. Kleinman, W.A. Nordland and A.C. Gossard, 1980. Luminescence studies of optically pumped quantum wells in GaAs-AlGaAs multilayer structures. *Phys. Rev.*, B22: 863-871.
- Miller, R.C., D.A. Kleinman, W.T. Tsang and A.C. Gossard, 1981. Observation of excited levels of excitons in GaAs quantum well. *Phys. Rev.*, B24: 1135-1136.
- Miller, R.C., Kleinman, D.A. and A.C. Gossard, 1984. Energy gap discontinuities and effective masses for GaAs-AlGaAs quantum wells. *Phys. Rev.*, B29: 7085-7087.
- Rogers, D.C. and R.J. Nicholas, 1985. Limit on band discontinuities in GaAs heterostructures deduced from optical photoresponse. *J. Phys. C. Solid State Phys.*, 18: 1891-1896.
- Schulman, J.N. and McGill, 1979. The CdTe/HgTe superlattices: Proposal for a new infrared material. *Appl. Phys. Lett.*, 34: 663-665.
- Schulman, J.N. and Y.C. Chang, 1985. Band mixing in semiconductor superlattices. *Phys. Rev.*, B31: 2056-2068.
- Schulman, J.N. and Y.C. Chang, 1983. Reduced Hamiltonian method for solving the tight-binding model interfaces. *Phys. Rev.*, B29: 2346-2354.
- Weisbuch, C., R.C. Miller, R. Dingle and A.C. Gossard, 1981. Intrinsic radiative recombination from quantum states in GaAs/AlGaAs multi-quantum well structures. *Solid State Commun.*, 37: 219-222.
- White, S.R. and I.J. Sham, 1981. Electronics properties of flat-band semiconductor heterostructures. *Phys. Rev. Lett.*, 47: 879-882.