Excitonic Emission of AlGaAs/GaAs Quantum Well Heterostructures

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Abstract: Excitonic Emission of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ Quantum Well with different contents of Al of (0.1 to 0.4) was studied theoretically. The investigation of excitonic emission of GaAs overgrown in AlGaAs matrix was calculated using the method of finite differences to find the one-dimensional band diagram of a semiconductor structure. Based on a solution of Schrödinger's equation, the program calculated the conduction and valence bands, and the hole and electron concentrations. The results of the calculations of the band gap of $Al_xGa_{1-x}As$ layers with different Al contents shows that with increasing Al content, the band gap of $Al_xGa_{1-x}As$ is increasing. The layers of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well were formed where AlGaAs acts as a barrier around GaAs which contribute to confinement of the carriers in GaAs layer. Our calculations observed that, this barrier height increasing with increasing of Al content from x=0.1 to 0.4.

Keywords: GaAs, AlGaAs, Quantum Well, Heterostructures

1 Introduction

Quantum wells are one example of heterostructures structures made by joining different materials, usually in layers, and with the materials joined directly at the atomic level. When two semiconductors are joined, it is not clear in advance how the different bands in the two materials will line up in energy with one another, and there is no accurate predictive theory in practice. Quantum wells are one example of heterostructures made by different materials layers. Hence, an important experimental quantity is the "band offset ratio"; this is the ratio of the difference in conduction band energies to the difference in valence band energies. Typical examples include growing thick GaAs [1] or AlGaAs layers [2,3] and a subsequent analysis of the intensity of their optical properties. For GaAs/AlGaAs heterostructures, for example, approximately 67% of the difference in the band gap energies is in the conduction band offset, and 33% is in the valence band offset, giving a ratio 67:33 [3,4]. In this material system, both electrons and holes see higher energies in the AlGaAs than in the GaAs, giving a so-called "Type I" system. They can be used for advanced electronic devices (e.g., modulation-doped field-effect transistors, heterojunction bipolar transistors, resonant tunneling devices), and optoelectronic devices and structures (e.g., laser diodes, photodetectors, quantum well and superlattice optical and optoelectronic devices) [4]. In the present article, we will introduce theoretical excitonic emission of AlGaAs/GaAs/AlGaAs quantum well. We will briefly allude to the different Al content of the outer layer and its effect on the band gap on the AlxGa1-xAs, then the effect of these changes of the band gap on the excitonic emission of the inner layer in detail.

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2 Theoretical Consideration and Calculations

Quantum size effects arise when the size of a nano-crystal is comparable to the length parameters i.e., the de Broglie wavelength λ and exciton Bohr radius aB of the quasi-particles (electrons, holes and excitons) [5].

$$\lambda=\frac{h}{p}=\frac{h}{\sqrt{3m^*_{e(h)}kT}} \qquad a_B=\frac{\hbar^2\varepsilon_\infty}{e^2}\left[\frac{1}{m^*_e}+\frac{1}{m^*_h}\right] \qquad (1)$$

where $m^*_{e(h)}$ is the effective mass of electron (hole), T is the temperature and h, k are Blank and Boltzmann constants, respectively. $\varepsilon\infty$ is the dielectric constant.

At room temperature, λ is around 10 nm. For most common semiconductors a_B is in the range of 1-10 nm which indicates that quantum size effects are pronounced even for a particle with dimension ten to hundred times larger than the lattice constant.

The real space stationary Schrödinger equation for an electron in a bulk crystalline solid with a spatially periodic potential is [6]

$$\left[\frac{-\hbar^2}{2m^*}\nabla^2+V(r)\right]\Psi(r)=E\Psi(r) \qquad (2)$$

where the first term represents the kinetic energy operator for the electron and V(r) is the periodic potential energy seen by the electron.

and $\Psi(r)$ is the wave-function.

In general, the potential V(r) may include the ionic potential as well as any electron-electron interactions. Since the potential is periodic with respect to lattice translations then the V(r) has the property:

$$V(r)=V(r+T) \qquad (3)$$

where T represents a lattice vector. The Bloch theorem indicates that an eigen-function of the Schrödinger equation for a periodic potential is the product of a plane wave $e^{ik.r}$ times a function $u_{v,k}(r)$ which has the same periodicity as the periodic potential. Thus, we get:

$$\Psi_{v,k}(r)=e^{ik.r}u_{v,k}(r) \quad (4)$$

and

$$u_{v,k}(r)=u_{v,k}(r+T) \quad (5)$$

Assuming a parabolic band, the eigenvalues of equation (5) for the eigenfunctions are given by [6]

$$E(k)=\frac{\hbar^2k^2}{2m^*} \quad (6)$$

with m^* being the effective mass of electron or hole.

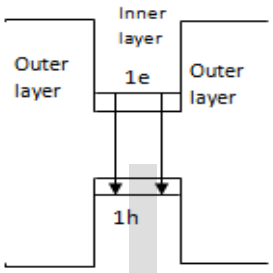


Fig. 1: Schematic diagram of optical transitions for type 1 quantum well.

There are three cases of the band alignment can be distinguished, denominated type-I, reverse type-I, and type-II band alignment [3]. In type-I, the shell is used to passivity the surface of the core with the goal to improve its optical properties. In reverse type-I systems, a material with narrower band-gap is overgrown onto the core with wider band-gap. Charge carriers are at least partially delocalized in the shell and the emission wavelength can be tuned by the shell thickness. The most extensively analyzed systems of this type are CdS/HgS, [7] CdS/CdSe [8] and ZnSe/CdSe [9]. In type-II systems, shell growth aims to a significant red-shift of the emission wavelength of the NCs. In the present work, type-I of the band-gap of the outer material is larger than that of the inner layer and both electrons and holes are confined in it as shown in figure 1.

3 Sample Configuration

The sample consisted of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well. The width of the sample is 20 nm/10 nm/20 nm as shown in figure 2.

4 Results and Discussion

The results of the calculations of the band gap of $Al_xGa_{1-x}As$ layers with different Al contents are shown in figure 3.

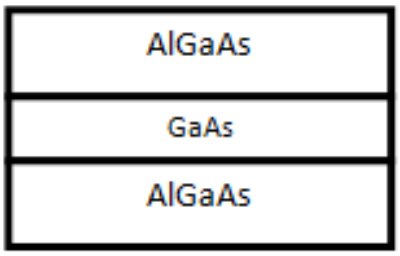


Fig. 2: Schematic diagram of the predicted sample structure.

It is observed form this figure that with increasing Al content, the band gap of $Al_xGa_{1-x}As$ is increasing. Suggest that there are layers of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well were formed. The AlGaAs acts as a barrier around GaAs which contribute to confinement of the carriers in GaAs layer. 1D Poisson program [10, 11] was used for calculation the conduction and valence bands, and the hole and electron concentrations. The program presents all of the quantized hole and electron states, whether they are occupied or not.

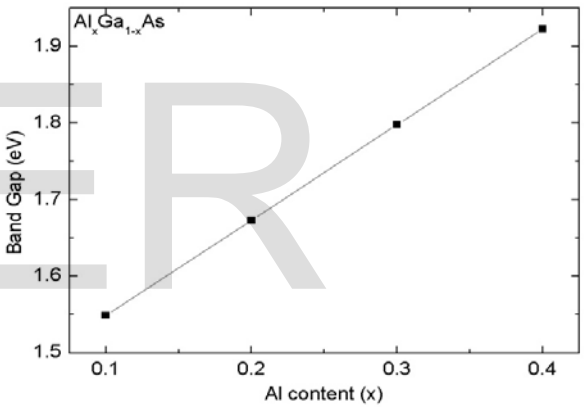
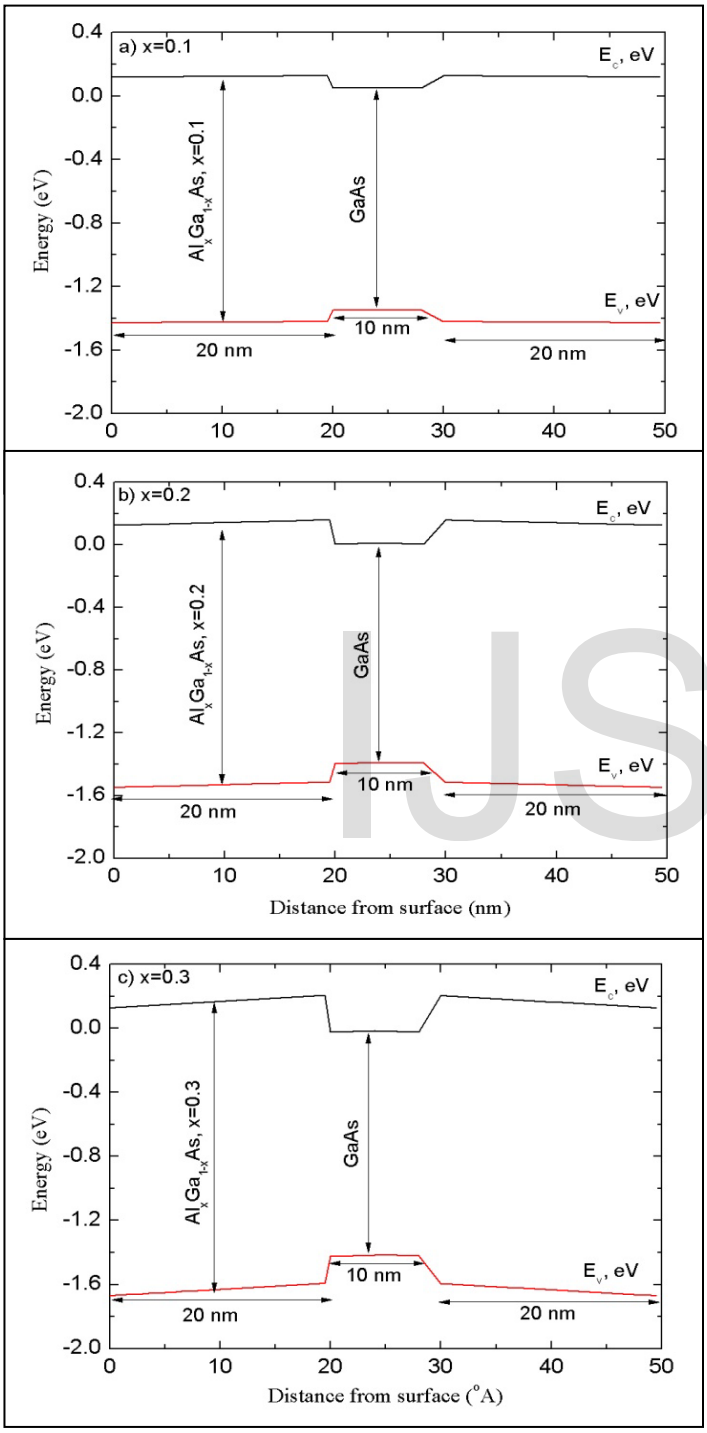


Fig. 3: The calculated band gap of $Al_xGa_{1-x}As$ with different values of Al content (x).

Figure (4) gives these resulting band structures used in the model calculations by 1D Poisson program for $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ with (a) x=0.1, (b) x=0.2, (c) x=0.3, and (d) x=0.4. Before presenting the results of the calculations, brief comments about the course of these calculations of the QW should be made. The starting GaAs thin layer has an average thin of 10 nm. As shown in figure (4), the 20 nm of AlGaAs acts like an outer layer around the GaAs thin layer. For overgrown GaAs in AlGaAs matrix, shown in figure (4a, b, c, and d), there is an increasing of Al content from x=0.1 to 0.4. This barrier height increasing with increasing of Al content from x=0.2 to 0.4. The shift between the energy levels of the GaAs in $Al_xGa_{1-x}As$ matrix as a function of Al content are calculated and plotted in figure (5). The results in the figure 5 clearly revealed that for the particular band offset, the eigenvalue of the inner layer increase as the well height increase of the outer layer. The observation is due to the fact that as the conduction band or the potential barrier height for the electron increases. Thus it is observed that the confinement energies of

the QW increase with the height of the potential barrier. The results of the calculated band structures are compared with experimental data of many workers. For all four types of $Al_xGa_{1-x}As$ outer layer, we find a quantitative agreement between experimental and calculated data.



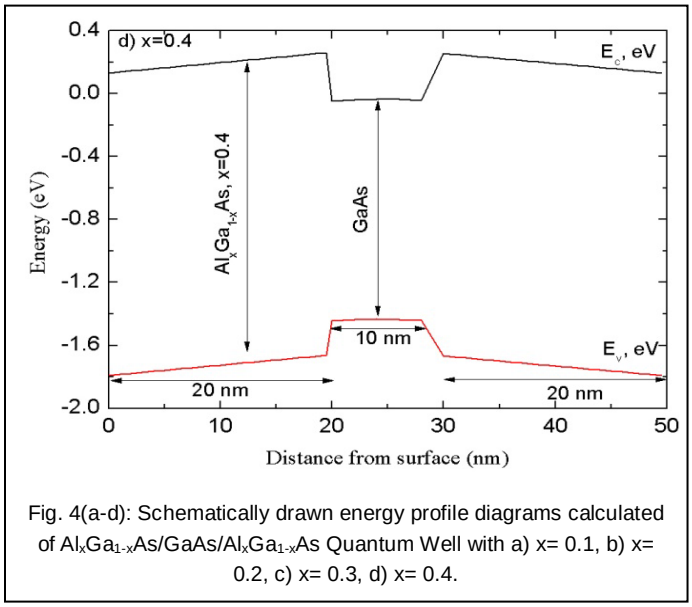


Fig. 4(a-d): Schematically drawn energy profile diagrams calculated of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ Quantum Well with a) x= 0.1, b) x= 0.2, c) x= 0.3, d) x= 0.4.

P. Acosta-Díaz et. al [12] presented results of a photoluminescence spectroscopy (PL) study of $Al_xGa_{1-x}As/GaAs$ QWs, x=0.3 grown by MBE on GaAs buffer layers. Their QWs exhibit drastic changes in their PL spectra depending on the type of interruption process performed on the GaAs buffer layer surface. They obtained an energy of 1.505 eV which is very close to the position of the first peak at 1.507 eV, therefore they assign this peak to the emission from the 5000 Å-thick GaAs buffer layer. Their experimental results is compared with the predication results calculated by our model at x=0.3. The difference between thier energy value comes from the difference of GaAs thickness

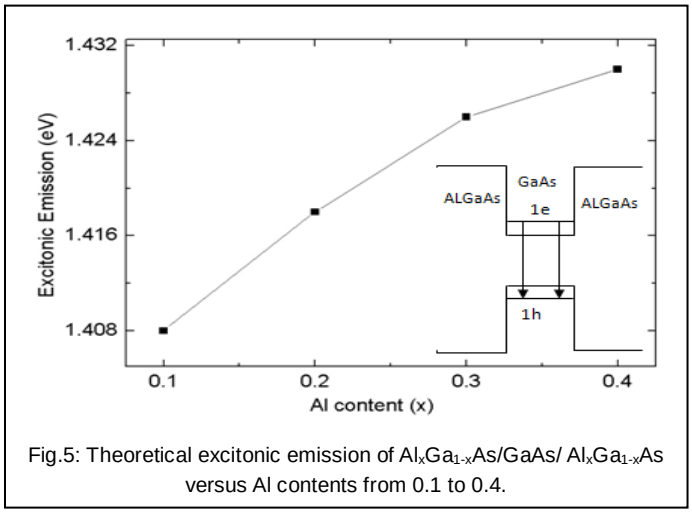


Fig.5: Theoretical excitonic emission of $Al_xGa_{1-x}As/GaAs/ Al_xGa_{1-x}As$ versus Al contents from 0.1 to 0.4.

Similar behavior is observed of type I Multiple Quantum Well (MQW) system of GaAs-AlGaAs grown by molecular beam epitaxy (MBE) by Ajayi Jonathan Olanipekun et. al. [13]. 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) of GaAs-AlGaAs system. The 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). It is revealed from their investigations that the confinement energies of the particles increase with increase in the height of the potential barrier for electron. The increase is more pronounced in the case of the light hole. However, these findings revealed clearly that the confinement energies of the particles vary as the band offsets. We consider this as a strong support of the assumptions made above indicating that GaAs incorporated in a AlxGa1-xAs matrix maintain their optical properties.

5 Conclusion

A matrix of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ QW with (a) x=0.1, (b) x=0.2, (c) x=0.3, and (d) x=0.4 is suggested. The conduction and valence bands, then the hole and electron concentrations are calculated. It is observed with increasing Al content, the band gap of $Al_xGa_{1-x}As$ is increasing. The AlGaAs barrier around GaAs contributes to confinement of the carriers in GaAs layer. The results of the calculated band structures are compared with experimental data of many workers. For all four types of $Al_xGa_{1-x}As$ QW with (a) x=0.1, (b) x=0.2, (c) x=0.3, and (d) x=0.4 outer layer, we find a quantitative agreement between experimental and calculated data.

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