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Aslan Turkoglu (✉ aslan.turkoglu@gmail.com)

: Researchers <https://orcid.org/0000-0002-4260-6217>

Yüksel Ergun

Eskişehir Technical University: Eskişehir Teknik Üniversitesi

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Investigation of the electro-optical characteristics of GaAs/AlGaAs multiple quantum well grown by metal organic vapor phase epitaxy

A. Türkoğlu¹ and Y. Ergün²

¹ Independent Researcher, Ankara, Turkey.

² Department of Physics, Faculty of Science, Eskişehir Technical University,
Eskişehir, Turkey.

ABSTRACT

In this study, the photoluminescence measurements of GaAs/Al_{0.25}Ga_{0.75}As multi-quantum-wells heterojunction structure grown on n⁺-GaAs substrates by Metal Organic Vapor Phase Epitaxy (MOVPE) method are investigated. By dropping 5145 Å wavelength laser light on the sample at room temperature and low temperatures, the transitions between the bands in the structure and the changes in these transitions under the different electric fields and temperatures are observed. In addition, by making theoretically developed self-consistent potential calculations, the subband energy levels and their corresponding wave functions of the structure under the electric field and without the electric field are calculated. The obtained numerical results were found to be in full agreement with the experimental measurements and theoretical calculations.

Keywords: Photoluminescence, Multiple Quantum Wells, Self-Consistent Calculation.

I. Introduction

There has been a growing interest in quantum well, quantum wire and quantum dot structures, which have more advantageous physical properties than those observed in bulk structures. The reduction of the dimensions in these quantum structures causes new physics and phenomena with potential electronic and optoelectronic device applications. The investigation of the luminescence properties of quantum well structures provide fundamental knowledge for manufacturing quantum well photoelectronic devices; such as quantum well lasers, quantum well photodetectors and quantum well photoconductive switches. However, many studies discuss the photoluminescence emission of GaAs / AlGaAs quantum wells [1-13].

The knowledge of exciton states is important for the correct understanding of some optical properties in the semiconductor low-dimensional systems. While no exciton resonance is observed in bulk semiconductors at room temperature, an exciton resonance can be observed even at room temperature in quantum wells. For this reason, the excitonic effects play an important role in the absorption and radiation spectra of GaAs/AlGaAs quantum wells. The electrical field dependence of optical absorption near the optical band edge in semiconductors is a major issue. In pure semiconductors, particularly at low temperature, the absorption edge in direct-gap semiconductors can be dominated by the exciton absorption resonances corresponding to the formation of an electron and hole in a hydrogenic orbit. Also, the electron and hole states in GaAs/AlGaAs quantum wells are affected by the application of electromagnetic fields, and also by external perturbations like temperature [14].

In doped structures, examining the effect of dynamic potential structure emerging due to the presence of free carriers is important in understanding the system. The shape of the considered potential defines the energy states of these carriers. Thus, the confining potential, the density profile, the subband energies, the subband occupations, and the Fermi energy in doped structures can be calculated self-consistently by the Schrödinger and Poisson equations [15]. On the other hand, in non-doped structures; there is no need to solve in a self-consistent way since the built-in potentials are previously known and fixed potentials.

In this study, the periodic 10 quantum well system with potential profiles shown schematically in Figure 1, will be considered. The confining potential profiles, electronic density profiles, subband energies, and subband localizations of GaAs/Al_{0.25}Ga_{0.75}As multiple quantum well are calculated by using the schematic representation in Figure 2. In addition, the effects of applied external static electric field and temperature on the optical properties of the structure were investigated experimentally by photoluminescence measurements. The organization of

this work is as follows: in the next section, we outline the theoretical formalism and experimental details used to investigate the electronic and optical properties of the system, and then in section 3, we introduce the obtained numerical results along with their physical comments. Finally, in section 4, we summarize our conclusions.

Figure 1. The confining potential profile of the conduction band of 10 periods GaAs multiple quantum well.

Figure 2. Schematic representation for the self-consistent calculation.

II. Theory

In this section, we will give general information about the self-consistent calculation technique that was used to calculate the electronic properties of the structure. The electronic structure of the system to be examined was created by using the effective mass and parabolic band approximations. We calculated the confining potential, the charge density, the subband energy levels, and their corresponding wave functions self-consistently by solving the Schrödinger and Poisson equations. The time-independent one-dimensional Schrödinger equation for an electron (a heavy hole or a light hole) confined in the conduction (valance) band of the structure can be written as [16]

$$\left(-\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V(z) \right) \psi_i(z) = E_i \psi_i(z) \quad (1)$$

Here, m^* represents the electron effective mass, $\hbar$ is Planck's constant, $V(z) = V_0(z) + V_H(z)$ is an effective potential, $V_0(z)$ is the confinement potential of the system, and $V_H(z)$ is the Hartree potential and is determined by the Poisson equation [17]

$$\frac{d^2 V_H(z)}{dz^2} = -\frac{4\pi e^2}{\epsilon} [N(z) - N_d(z)] \quad (2)$$

where ϵ is the GaAs dielectric constant and $N_d(z)$ is the total density of ionized dopants. The electron density is related to the electronic wave functions by the relation

$$N(z) = \sum_{i=1}^{n_d} n_i |\psi_i(z)|^2 \quad (3)$$

where n_d is the number of filled states, n_i represents the temperature-dependent number of electrons per unit area in the i th subband given by

$$n_i = \frac{m^* k_B T}{\pi \hbar^2} \ln \{ 1 + \exp[(E_F - E_i)/k_B T] \}. \quad (4)$$

and at $T = 0$ K, the above equation becomes as follows

$$n_i = \frac{m^*}{\pi \hbar^2} (E_F - E_i) \quad (5)$$

where i shows subband index, k_B is Boltzmann constant and E_F is Fermi energy. All donors are assumed to be ionized in calculations. The self-consistent solution of Eqs. (1)–(5) gives the confining potential profile, the subband energy levels, and their corresponding wave functions. The physical constants used in this study are as follows [18]: $m^* = 0.067m_0$, $m_{hh} = 0.45m_0$, $m_{lh} = 0.082m_0$, (m_0 is the free electron mass), $e = 1.602 \times 10^{-19}$ C, $\hbar = 1.056 \times 10^{-34}$ Js, $L_w = 50\text{\AA}$, $L_B = 100\text{\AA}$, $\varepsilon = 12.58$, $V_0 = 200\text{meV}$.

III) EXPERIMENTAL DETAILS

In this study, the structure of GaAs/AlGaAs multiple quantum wells are shown in Figure 3. First, $1\mu\text{m}$ thick n^+ – GaAs ($1 \times 10^{18}\text{cm}^{-3}$) layer is grown on the substrate. However, the undoped and symmetrical AlGaAs barrier is constructed in three steps:

- i) An inclined layer of $500\text{\AA}$ in which x is increased from 0 to 0.25,
- ii) Central $\text{Al}_{0.25}\text{Ga}_{0.75}\text{As}$ region with a width of $1400\text{\AA}$ containing 10 periods GaAs multiple quantum wells,
- iii) An inclined layer of $500\text{\AA}$ in which x is reduced from 0 to 0.25.

$1\mu\text{m}$ thick n^+ – GaAs ($1 \times 10^{18}\text{cm}^{-3}$) layer is added on the upper side.

Figure 3. Sample structure.

Using the experimental setup in Figure 4, a laser light of $5145 \text{ \AA}$ is dropped on the sample consisting of 10 periods GaAs multiple quantum wells at 65 K, and thus the electrons in the valence band are excited to the conduction band. The peaks in the photoluminescence spectrum observed as a result of the recombination of these excited electrons by various mechanisms and the corresponding transition energies are investigated. The spectra to be examined separately below are obtained by counting the light, which is released from the recombination of the excited electrons, by means of the detector.

Figure 4. Schematic representation of the experimental setup.

In Figure 5, the theoretically calculated wave functions for the electron, heavy hole, and light holes at 65 K are shown. As can be seen from the figure, in the absence of an external electric field, it is seen that the charge carriers are equally likely in each well.

Figure 5: The electronic wave functions and confining potential for (a) electron, (b) heavy hole, and (c) light hole in the absence of an electric field at 65 K.

The structure includes 50 Å GaAs multiple quantum wells and 100 Å AlGaAs barrier layers surrounding them. The photoluminescence spectrum observed as a result of the recombination of the excited electrons with various mechanisms is shown in Figure 6. The spectrum is obtained by counting the light released during the reunion processes of the excited electrons by means of the detector. In addition, the numerical values of the electron, heavy hole, and light hole ground state energy levels obtained as a result of theoretical calculations are presented in Figure 7. It is seen that the peak values seen in the spectrum and the transition energies obtained in the calculations are completely consistent with each other.

Figure 6: Photoluminescence spectrum observed in the absence of an electric field at 65K.

Figure 7: At 65 K, the schematic representation of the theoretically calculated energy levels for electron, heavy hole, and light hole in absence of external applied electric field.

In Figure 8, the peaks in the observed different photoluminescence spectrum and the corresponding transition energies are examined. As seen in Figure 7, at 65K, while no electric field is applied to the sample ($V=0$); the ground state energy levels calculated theoretically with the self-consistent calculation for the electron, light hole, and heavy hole are found to be 75 meV, 49 meV and 25 meV, respectively. Considering that the forbidden energy interval value calculated for the GaAs is 1.510 eV, it is understood that e1-lh1 transition corresponding to 1.636 eV in Figure 8 is a free exciton transition. Thus, it can be concluded that the e1-lh1 transition energy corresponding to 1.636 eV is a free exciton transition. This value equals to the sum of the encirclement energies of e1-lh1 pairs obtained by self-consistent calculation for GaAs / $\text{Al}_{0.25}\text{Ga}_{0.75}\text{As}$ and the forbidden energy range of GaAs are given as follows

$$E_{e1-lh1} = E_{GaAs} + E_{e1} + E_{lh1}. \quad (6)$$

The second peak corresponding to 1.617 eV shows that e1-hh1 is a free exciton transition:

$$E_{e1-hh} = E_{GaAs} + E_{e1} + E_{hh1}. \quad (7)$$

On the other hand, e1-hh1 that is the bound exciton:

$$E_{e1-hh1} = E_{GaAs} + E_{e1} + E_{hh1} - E_{exc}(e1 - hh1). \quad (8)$$

$E_{exc}(e1 - hh1)$ value is around 15 meV for a quantum well of 50 Å width [18,19]. When these values are taken into consideration, it can be seen that the third peak value in Figure 8 is e1-hh1 that is the bound exciton transition.

Figure 8: Peak values corresponding to spectrum and transitions observed at 65 K in the absence of an external electric field.

Figure 9: The electronic wave functions and confining potential for (a) electron, (b) heavy hole, and (c) light hole in the presence of an electric field (200 mV) at 65 K.

Figure 10: Photoluminescence spectrum observed in the presence of an electric field (200 mV) at 65K.

Figure 11: At 65 K, the schematic representation of the theoretically calculated energy levels for electron, heavy hole, and light hole in the presence of external applied electric field (200 mV).

Figure 12: Peak values corresponding to spectrum and transitions observed at 65 K in the presence of electric field (200 mV).

The wave functions calculated under 65 K and 200 mV voltage are shown separately for electron, heavy hole, and light hole in Figure 9. Also, the photoluminescence spectrum is given in Figure 10. In Figure 11, the electron and hole energy level values obtained as a result of the voltage applied to the sample are presented. When these calculated values are written in the following expression

$$E_{e1-lh1} = E_{GaAs} + E_{e1} + E_{lh1} = 1.510 + 0.068 + 0.047 = 1.625 \text{ eV} \quad (9)$$

Considering the theoretically calculated e1-lh1 free exciton transition energy value, it can be concluded that the transition corresponding to 1.626 eV in Figure 11 is e1-lh1 free exciton transition. Similarly, e1-hh1 transition energy value is obtained as follows

$$E_{e1-hh1} = E_{GaAs} + E_{e1} + E_{hh1} = 1.510 + 0.068 + 0.022 = 1.600 \text{ eV}. \quad (10)$$

As can be seen from Figure 12, this value corresponds to the peak value of 1.605 eV in the photoluminescence spectrum. In Figure 11, E_{e1-hh} (bound excitation) is equal to 1.585 eV. Here, it can be said that the transition corresponding to 1.588 eV in Figure 12 is e1-hh1 that represents bound exciton transition.

Figure 13: The electronic wave functions and confining potential for (a) electron, (b) heavy hole, and (c) light hole in the presence of an electric field (400 mV) at 65 K.

Figure 14: Photoluminescence spectrum observed in the presence of an electric field (400 mV) at 65K.

Figure 15. At 65 K, the schematic representation of the theoretically calculated energy levels for electron, heavy hole, and light hole in the presence of external applied electric field (400 mV).

Figure 16: Peak values corresponding to spectrum and transitions observed at 65 K in the presence of electric field (400 mV).

Under 400 mV voltage, the wave functions of electron, heavy, and light holes are given in Figure 13 and the observed photoluminescence spectrum is given in Figure 14. Finally, the energy level values of electrons and holes are shown in Figure 15. It can be easily seen from Figure 15 that E_{e1-hh} , E_{e1-lh1} and E_{e1-hh1} (bound exciton) are obtained as 1.616, 1.596 and 1.581 eV, respectively. According to these transition energies, in Figure 16, the free exciton transition e1-lh1 (electron-heavy vacuum) of the first transition corresponds to 1.618 eV and e1-lh1, which is the free exciton energy of the second transition, corresponds to 1.593 eV. It can be seen that the third transition corresponds to 1.576 eV, which also corresponds to e1-hh1 bound exciton transition. The binding energy of Carbon acceptors in the bulk structure is approximately 22 meV [21]. In GaAs quantum wells, this value was found to be approximately 32 meV [22]. The following expression can be written for the e1-A(C) transition energy

$$E_{e1-A(C)} = E_{GaAs} + E_{e1} + E_{hh} - E_{A(C)} = 1.510 + 0.062 + 0.019 - 0.032 = 1.559 \text{ meV}.$$

In Figure 16, we can say that the transition corresponding to 1.559 eV is the transition of e1-A(C).

Figure 17. Comparison of the experimental results observed for the change with voltage of the transition energies from the conduction band to the valence band with the values found by theoretical calculation.

In Figure 17, the experimentally observed values and the values found by theoretical calculations for the e1-lh1 free exciton transition energies, e1-hh1 free exciton transition energies, e1-hh1 connected exciton transition energies, and e1-A (C) transition energies in the photoluminescence spectrum are given on the same graph. As can be seen from the figure, the experimental results are consistent with the theoretical calculations.

Figure 18: Photoluminescence observed under different voltage values comparative graph of normalized spectra.

In Figure 18, the photoluminescence spectra observed under different voltage values at 65K temperature are normalized and shown comparatively. It is observed that as the voltage value increases, the spectra, thus the peaks, shift to the left in the energy axis. In other words, the higher the voltage value, the smaller the peak energy values. The reason for this is that the values of the subband energy levels decrease and the energies of the transition from the conduction band to the valence band decrease due to the increment of the confining potential in the quantum wells under the electric field.

Figure 19: The variation of photoluminescence spectra with the temperature in the absence of electric field.

Finally, the photoluminescence spectra observed at different temperature values are given in Figure 19. Here, the voltage is not applied to the sample, only the temperature is increased. As can be seen from this figure, as the temperature value increases, the photoluminescence spectra shift to the left in the energy axis and the transition energies decrease. In addition, the intensity of photoluminescence decreases with the increasing temperature. According to the equation of $E_g(T) = E_0 - \left(\frac{\alpha T^2}{T+\beta}\right)$ (Here, $E_0 = 1.519$ eV, $\alpha = 5.405 \times 10^{-4}$ and $\beta = 204$ K) [23]; as the temperature increases, the GaAs forbidden energy range will decrease. In other words, electrons will gain a smaller energy as they move from the energy levels in the valence band to the energy level in the conduction band, and hence they will emit photon with a smaller energy as they move to the valence band for recombination. Therefore, a decrease in transition energies is an expected result. However, with the increasing temperature, the intensity of photoluminescence also decreases; as lattice vibrations and phonon scattering come into play.

CONCLUSIONS

A laser light of 5145 Å wavelength using Ar laser source is dropped on 10 periods GaAs/Al_{0.25}Ga_{0.75}As quantum wells and the photoluminescence measurements are made. For different temperature values, starting from 65 K, the effect of temperature change on the recombination mechanisms in a multi-quantum well structure and thus on the photoluminescence spectrum is investigated. A decrease in the energy and intensity of light released in the recombination mechanisms is observed with the increasing temperature values. The reason for this situation is the lattice vibrations that increase with the temperature increment and the decrement of the GaAs forbidden energy range. Then, by holding the temperature constant, different values of voltage are applied and the effect of applied voltage on photoluminescence measurements is examined. It is observed that with the increasing voltage, the energy of the released light decreased while its intensity increased. The decrease in the energy of light, the decrease in energy levels in multi-quantum well structure with the applied voltage, and the increase in intensity are due to the increase in the number of excited electrons. The obtained findings were compared with theoretical calculations, and it was seen that the experimental results were in full agreement with the theoretical results. In conclusion, the numerical results are extremely important in terms of understanding the excitonic transitions in these structures.

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