THE STRUCTURE PARAMETER EFFECTS ON THE ELECTRONIC AND OPTICAL PROPERTIES OF GAUSSIAN SHAPED DOUBLE QUANTUM WELLS UNDER ELECTRIC FIELD

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Abstract

Infrared detecting Gaussian shaped $Al_xGa_{1-x}As/\ GaAs/\ Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ double quantum wells have been designed. The energy states and the electronic wave functions have been calculated by the finite difference method within the effective mass approximation. The structure parameter, which design the potential profile of the device, was increased to explore its effect on the first for energy states at different electric field strength. The results showed that increase in the electric field strength shift the peak values of the total absorption coefficients to smaller photon energies, meaning a blue shift.

Keywords: Double quantum well, energies, optical absorption coefficient

INTRODUCTION

Electronic and optoelectronic devices such as diodes and transistors are produced from semiconductor crystals, and such device types in which the movements of charge carriers are dimensionally limited are examined and produced under the name of low-dimensional structures [1,2]. The electronic and optical properties of low-dimensional structures that can be customized as quantum wells, quantum wires and quantum dots continue to be a very important research area due to their technological importance [3-7].

Studies have reported how the shapes of double quantum wells and applied external fields affect their energy states [8–14]. How the barrier width between the quantum well pair changes the electronic properties of the structure has been showed [8]. It has been found that the correct well widths and barrier height in asymmetric double semi-V-shaped quantum wells provide the desired optical properties of the structure [12]. Kasapoglu et al. have calculated the energy states and wave functions in the symmetric and anti-symmetric Gaussian quantum wells under external laser and magnetic fields. They have showed the variations of total absorption coefficients and total reflection indices for allowed transitions depending on the photon energy, and stated that by selecting appropriate structural parameters, the electronic and optical properties of the structures can be controlled by external fields [13,14].

In the light of these studies, we theoretically consider a Gaussian-shaped double quantum well (GSDQW) in composition of $Al_xGa_{1-x}As\ /\ GaAs\ /\ Al_xGa_{1-x}As\ /GaAs\ /\ Al_xGa_{1-x}As$. First, the energy states and wave functions were calculated depending on the structural parameters under electric field. Then, the total absorption coefficients for the (2-3) transitions which depend on the electric field intensity and photon energy were obtained.

THEORY

The time independent Hamiltonian of an electron, in the units of effective Bohr radius $a^* = \varepsilon\hbar^2/me^2$ and Rydberg energy $R^* = me^4/2\hbar^2\varepsilon^2$ is given by

$$H = -\nabla^2 + V(z) \quad , \qquad (1)$$

where $V(z)$ the potential energy of GSDQW which can be expressed as

$$V(z) = V_0 \begin{cases} \dfrac{1}{e^{-\frac{(z+L_z)^2}{c}} + e^{-\frac{(z)^2}{c}} + e^{-\frac{(z-L_z)^2}{c}}} & |z| \geq Lz \\ elsewhere \end{cases} . (2)$$

In Eq.2, V_0 is the barrier height, L_z is the half of total width of structure at V_0 level, and c is the parameter whom draws the shape of GSDQW. When an electric field is applied, Eq.1 takes the form of

$$H = -\nabla^2 + V(z) + \eta z \quad , \quad (3)$$

where $\eta = |e|Fa^*/R^*$ is the the potential of electric field applied in the $+z$-direction. If the eigenfunction of the Hamiltonian in Eq. (3) is represented as $\varphi_n(\mathrm{z})$, the Schrödinger equation can be given as

$$\frac{d^2\,\varphi_n(\mathrm{z})}{dz^2} + [E_n - V(z) - \eta z]\,\varphi_n(\mathrm{z}) = 0 \quad , \quad (4)$$

from which the energy levels E_n and wavefunctions $\varphi(\mathrm{z})$ can be found by using the finite differences method [3].

For a z-polarized incident radiation, the dipole transition matrix between initial state *i* and final state *j* is given by

$$M_{ij} = \langle \varphi_i | ez | \varphi_j \rangle \quad (5)$$

The total optical absorption coefficients $\beta(\omega, I)$ for the electronic polarization as a response to an electromagnetic field with frequency ω is [15-17].

$$\beta(\omega, I) = \beta^1(\omega) + \beta^3(\omega, I) \quad , \quad (6)$$

where the linear and nonlinear optical absorption coefficients $\beta^1(\omega)$ and $\beta^3(\omega, I)$ are

$$\beta^1(\omega) = \frac{\sigma}{\epsilon_0 n_r c} \frac{|M_{ij}|^2 \hbar\omega\Gamma}{(E_{ij} - \hbar\omega)^2 + (\hbar\Gamma)^2} \quad , \quad (7)$$

and

$$\beta^3(\omega, I) = -\left(\frac{2I\sigma}{[\epsilon_0 n_r c]^2}\right) \frac{|M_{ij}|^4 \hbar\omega\Gamma}{[\,(E_{ij} - \hbar\omega)^2 + (\hbar\Gamma)^2]^2} . (8)$$

as expressed previously [15-17]. In Eqs.7 and 8 n_r is the refractive index, Γ is the relaxation coefficient, I is the optical intensity of the incident wave [6, 18]. The transition energy E_{ij} is given by

$$E_{ij} = E_j - E_i \quad , \quad (9)$$

and defined as the energy difference between the final E_j and initial states E_i.

RESULTS

In a general framework, in this study, the electronic and optical properties of the Gaussian shaped quantum well pair structure were examined for two values of the structure parameter c, without and with an electric field. The calculations were for $L_z = 100$ Å and $V_0 = 228meV$. The other structural constants are, the Rydberg energy $R^* = 5.21$meV, the effective Bohr Radius $a^* = 105$ Å, the electron density $\sigma = 3x10^{22}m^{-3}$, the refractive index n_r=3.5, the relaxation coefficient of $\Gamma = 7.14x10^{12}\ s^{-1}$, and the optical intensity of $I = 400\ MW/m^2$ [19, 20].

In Figure 1a, for two values of the structure parameter, $c = 55$ Å^2 and $c = 495$ Å^2, the first two energy levels and the electronic wave functions at these levels are shown on the GSDQW potential profile. Figure 1b shows the results of applying an electric field of $F = 40\ kV/cm$ on the physical properties examined in Figure 1a. While quantum wells have a square well profile for $c = 55$ Å^2, by increasing the structure parameter value to $c = 495$ Å^2, the wells take the form of a parabolic profile. It has also changed from having narrow barrier to the Gaussian barrier profile. When the first two energy levels are examined in the both figures, they are close to each other. This is an expected behavior as the profile resembles a symmetric double quantum well. Increasing the structure parameter c increases the energy levels closing them each other. When an electric field was applied E_1 energy decreased while E_2 energy increased. φ_1 localizes in the left-hand side well for both c values, while φ_2 was

localized in the right-hand sight well if the electric field is on.

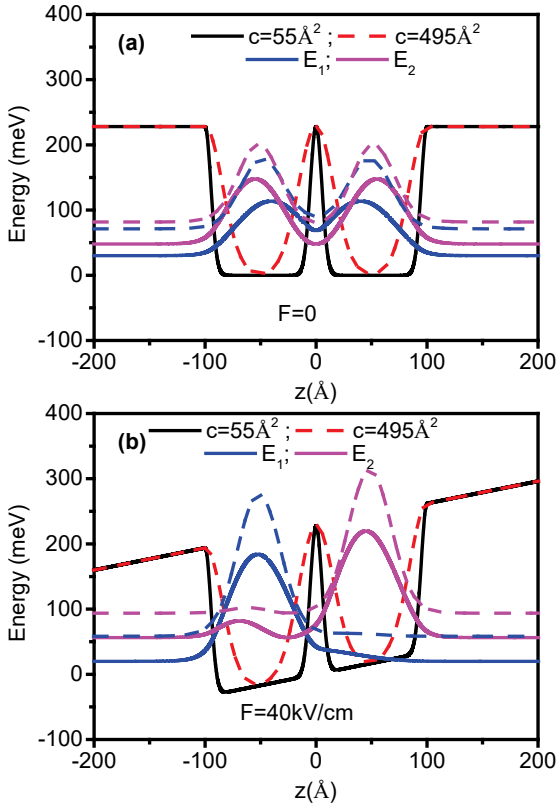

***Fig 1**. Gaussian double quantum well potential and probability densities corresponding to the first two energies for **(a)** F=0 and **(b)** F=40kV/cm at $c = 55$ Å^2 and $c = 495$ Å^2.*

The first four energy levels depending on the structure parameter c for no-field $F = 0$ and the field application of $F = 60\ kV/cm$ are shown in Figs. 2a, and 2b, respectively. While the E_1 and E_2 present slow linear increase by increasing the structure parameter c for $F = 0$, the E_3 and E_4 tend to level up for high c values. As can be seen in Fig.2b, with the application of an electric field of 60 kV/cm, depending on c, E_1 and E_2 do not show a significant difference compared to their characteristic behavior in the absence of electric field. However, the E_1 level decreases to lower energies. On the other hand, E_2 level increases. While the E_3 level is maintained, it rises and its levels up shifts to lower c values. In E_4, both a level decrease and a minimum at the middle values of c are observed.

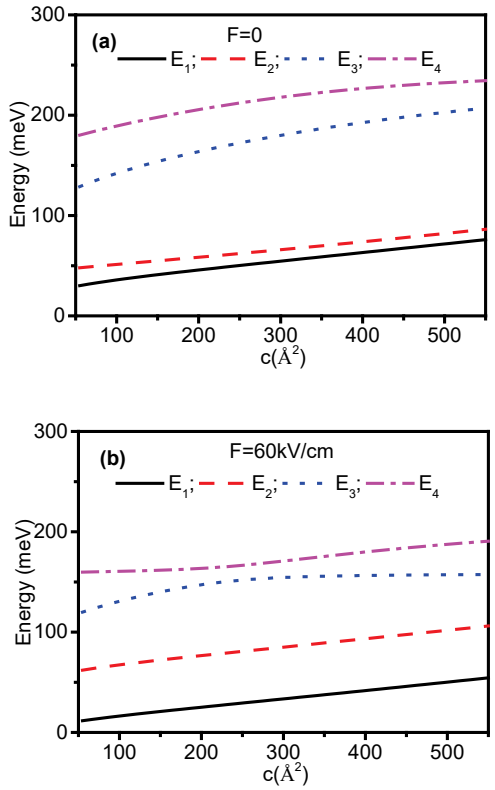

***Fig. 2.** Energy changes depending on the c parameter of the electron confined in the GSDQW under electric fields of (a) F=0, and (b) F=60 kV/cm, respectively.*

How these variations in the energies affect the transitions are shown in Fig.3 for (1-2), (1-3) and (2-3) transition energies under various the electric field strengths and no-field depending on the structure parameter c. (2-3) energy differences were observed to be higher compared to other transitions. It was observed that increasing the structure constant c in other transitions was not very effective.

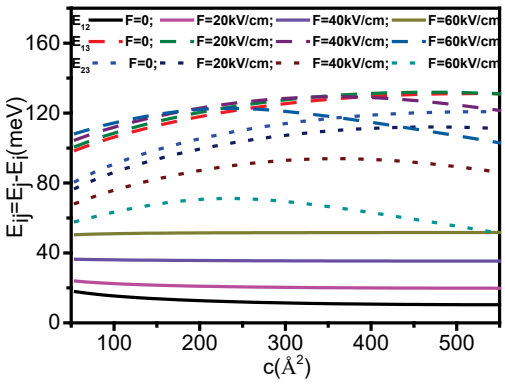

***Fig 3.** Variation of transition energies depending on the structure parameter c under various the electric field strengths.*

For the $c = 55$ Å^2, the total absorption coefficient variation of the (2-3) transition depending on the electric field strength and photon energy is given in Fig.4. It was observed that when the electric field was applied, the maximum values of the total absorption coefficient shifted to smaller photon energies. The source of this result is the resonance condition $\hbar\omega_{max} = \sqrt{(E_{ij} - \hbar\omega)^2 + (\hbar\Gamma)^2}$ given in Eq.7. The transition energy E_{ij} affects the total absorption coefficient. When the transition (2-3) given in Fig.3 is examined, it is seen that it decreases as the electric field increases. Another interesting point in Fig.4 is that the total absorption coefficient value, which is maximum when there is no electric field, decreases with the increasing electric field. Similar results have been seen in the concerning literature [21].

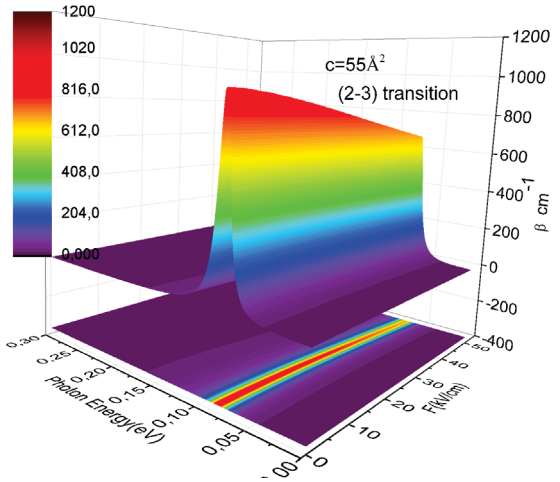

Fig 4. *For the $c = 55$ Å^2, the total absorption coefficient variation of the (2-3) transition depending on the electric field strength and photon energy.*

For $c = 495$ Å^2, the total absorption coefficient variation of (2-3) transition depending on electric field strength and photon energy is given in Fig.5. Increasing the c , the total absorption peak value shifts to higher photon energies for (2-3) transition. This means red shift. The maximum value of the total absorption coefficient was 1100 cm^{-1} in the field-off case, and it was rapidly decreases with the increasing electric field strength. Accordingly, the peak values shift to lower photon energies.

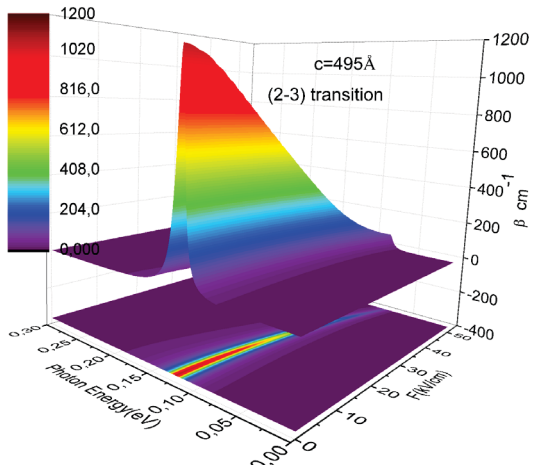

Fig 5. *For the $c = 495$ Å^2, the total absorption coefficient variation of the (2-3) transition depending on the electric field strength and photon energy.*

CONCLUSION

By changing the structure parameter c in the designed double quantum well separated by a Gaussian barrier potential, the first four energy levels and wave functions were calculated under the electric field. While the structure parameter change was not effective for the first two energy levels in the absence of an electric field, it was observed that it was effective for the 3rd and 4th energy levels. all energy levels affected in different ways depending on the electric field intensity. Furthermore, the total absorption coefficients in transition (2-3) were obtained as a function of photon energy and electric field intensity for two different structure parameters. It was observed that the increase in the structure parameter caused the total absorption coefficient to give a maximum at larger photon energies, and these energies occurred at infrared wavelengths. For both structures studied, a blue shift was observed in the maximum values of the total absorption coefficients when the electric field was applied. It was observed that the externally applied electric field changed the optical absorption spectrum. We believe that these results may be important for devices operating using in-band transitions.

REFERENCES

[1] Albo, A., Fekete, D., Bahir, G. Photocurrent spectroscopy of intersubband transitions in GaInAsN/(Al)GaAs asymmetric quantum well infrared photodetectors. J. Appl. Phys. 2012; 112: 084502.

[2] Peralta, X.G, Allen, S.J., Wanke, M.C., Harff, N.E., Simmons, J.A., Lilly, M.P., Reno, J.L.; Burke, P.J., Eisenstein, J.P. Terahertz photoconductivity and plasmon modes in double-quantum-well field-effect transistors. Appl. Phys. Lett 2002; 81: 1627–1629.

[3] Boz F.K., Aktas S., Bekar B., Okan S.E. Laser field-driven potential profiles of double quantum wells. Phys. Lett. A 2012 ; 376: 590-594.

[4] Sucu S., Minez S., Erdogan I. Self-polarization of a donor impurity for the first excited state in an Ga1-xAlxAs/GaAs quantum well. Indian Journal of Physics, 2021; 95:1691–1695.

[5] Rani, P., Dalal, R., & Srivastava, S. Study of electronic and optical properties of quantum dots. Applied Nanoscience, 2022; 12: 2127–2138.

[6] Bekar, B., Boz, F. K., Aktas, S., & Okan, S. E. The Effect on the Optical Absorption Coefficients due to the Positions in the Plane of Square GaAs / Al(GaAs) Quantum Well Wire under the Laser Field. Acta Physica Polonica A 2019; 136(6):882-888.

[7] Rani, P., Dalal, R., & Srivastava, S. Study of electronic and optical properties of quantum dots. Applied Nanoscience, 2022; 12: 2127–2138.

[8] Ozturk O, Ozturk, E.,Elagoz, S. The effect of barrier width on the electronic properties of double GaAlAs/GaAs and GaInAs/GaAs quantum wells. Journal of Molecular Structure 2018; 1156:726-732.

[9] Tanimu A., Muljarov E. A. Resonant states in double and triple quantum wells. J. Phys. Commun. 2018; 2: 115008.

[10] Kasapoglu E., Sakiroglu S., Sari H., Sökmen I., Duque C.A. Binding energy and optical absorption of donor impurity states in “12-6” tuned GaAs/GaAlAs double quantum well under the external fields. Physica B: Condensed Matter 2019; 554: 72-78.

[11] Karabulut İ., Mora-Ramos M.E., Duque C.A. Nonlinear optical rectification and optical absorption in GaAs–Ga1–xAlxAs asymmetric double quantum wells: Combined effects of applied electric and magnetic fields and hydrostaticpressure. J. Lumin. 2011; 131: 1502-1509.

[12] Yesilgul U., Ungan F., Kasapoglu E., Sari H., Sökmen I. Linear and nonlinear optical properties in asymmetric double semi-V-shaped quantum well. Physica B: Condensed Matter 2015; 475:, 110-116.

[13] Kasapoglu E., Yücel M. B., Duque C. A., Harmonic-Gaussian Symmetric and Asymmetric Double Quantum Wells: Magnetic Field Effects. Nanomaterials 2023; 13: 892.

[14] Kasapoglu E., Yücel M. B., Duque C. A., Parabolic-Gaussian Double Quantum Wells Under a Nonresonant Intense Laser Filed. Nanomaterials 2023; 13: 1360.

[15] Kaya D., Yücel M. B., M. B. Bayrak M. B. The total absorption coefficient and refractive index change of a spherical quantum dot in the confinement radial potential. Physica B: Condensed Matter 2023; 648: 414403.

[16] Ungan F., Yesilgul U., Kasapoglu E., Sari H., Sökmen I. The effects of hydrostatic pressure and intense laser field on the linear and nonlinear optical properties of a square quantum well. Optics Communications 2012; 285: 373-377.

[17] Ozturk O., Ozturk E., Elagoz S. Linear and nonlinear optical absorption coefficient and electronic features of triple GaAlAs/GaAs and GaInAs/GaAs quantum wells depending on barrier widths. Optik 2019;180: 394-405.

[18] [2036] En-nadir, R., El Ghazi, H., Belaid, W., Abboudi, H., Jabouti, F., Jorio, A., & Zorkani, I. The Confinement Profile Effect on the Optical Properties in Different Inverseshaped Single InGaN/GaN Quantum Wells. Iraqi Journal of Physics, (2022). 20(1): 1-13.

[19] [2137] Kavruk A. E., Sahin M., Atav Ü. A detailed investigation of electronic and intersubband optical properties of AlxGa1-xAs/Al0.Ga0.7As/AlyGa1-yAs/Al0.3Ga0.7As multi-shell quantum dots. J. Phys. D: Appl. Phys. (2014) ; 47(295302):1-8.

[20] Al E. B., Kasapoglu E., Sakiroglu S., Sari H., Sökmen I., Duque C. A. Binding energies and optical absorption of donor impurities in spherical quantum dot under applied magnetic field. Physica e (2020); 119(114011):1-8.

[21] Yesilgul U., Al E. B. , Martınez-Orozco, J. C. , Restrepo R. L., Mora-Ramos M. E. , Duque C. A., Ungan F., Kasapoglu E. Linear and nonlinear optical properties in an asymmetric double quantum well under intense laser field: Effects of applied electric and magnetic fields. Optical Materials (2016); (58): 107-112.