Journal of Basics and Applied Sciences Research (JOBASR)
ISSN (print): 3026-9091, ISSN (online): 1597-9962
Volume 3(4) July 2025
DOI: https://dx.doi.org/10.4314/jobasr.v3i4.2

Theoretical Analysis of Intersubband Optical Absorption in GaAs/AlGaAs Quantum Wells: Influence of Well Width and Dephasing Energy

Abubakar T. S.[1*], Faragai I. A.[2], Bichi T. S.[3] & Usama Bello[4]
[1,2,3,4]Department of Physics Aliko Dangote University of Science and Technology, Wudil
[*]Corresponding Author Email: turadsuraj@yahoo.com

ABSTRACT
This study presents a simulation of the optical absorption spectra within the THz frequency region using Matlab, considering a doping concentration of N=1×1040 cm^{-3}. Quantum well (QW) widths of 25 nm, 30 nm, 35 nm, and 40 nm were analyzed, with results depicted in Figures 11 through 14, respectively. The simulations incorporate varying dephasing energies Γ of 8 meV, 12 meV, and 16 meV to account for broadening mechanisms such as phonon interactions, impurity scattering, and other dephasing processes. A clear redshift in the absorption edge is observed with increasing QW width, as evidenced in results, indicating that wider wells accommodate lower energy confinement states. Additionally, the absorption peaks become sharper as the QW width increases, consistent. The dephasing energy significantly influences the spectral line shape; higher Γ values result in broader absorption features with diminished peak intensity, reflecting increased scattering and reduced electronic coherence. Conversely, lower Γ (8 meV) yields sharper peaks, aligning with previous experimental research by scholars. These results underscore the critical role of QW dimensions and dephasing mechanisms in tailoring the optical properties of quantum wells, which is essential for optimizing THz optoelectronic devices.

Keywords:
Intersubbands,
Dephasing Energy,
Terahertz,
Quantum well,
Optical Absorption.

INTRODUCTION

Substantial research efforts over many years have explored the relationship between light and material excitations, a topic that still draws considerable researcher attention (Jr & Faragai, 2014).

This field of study started with atomic physics and molecules, moved on to semiconductor systems, and has found effective applications in photonics and optoelectronics. It also makes it possible to examine a wide range of physical phenomena (Pereira & Faragai, 2013).

Intersubband transitions have delivered remarkable applications. Photonic devices such as quantum cascade lasers (QCLs) (Liu et al., 2024), quantum well infrared detectors (QWIP) (Zhang et al., 2024), and terahertz polariton emitters (C. H. Wu et al., 2023) are among the successful applications. Optical properties in quantum well semiconductors are a fascinating area of study. In quantum wells, the confinement of particles leads to quantized energy levels, which in turn affect the absorption and emission of light (Albo et al., 2012). This phenomenon plays a crucial role in the development of optoelectronic devices such as lasers and light-emitting diodes (Liu et al., 2024). Understanding the optical properties of quantum well semiconductors is essential for advancing technology in the field of photonics (Redaelli et al., 2015).

This paper studied intersubband optical absorption in GaAs/AlGaAs quantum wells: influence of well width and dephasing energy.

MATERIALS AND METHODS

Considering a P-type conduction band of n12=1.2 interacting with phone energy E_n

$$E_n = \frac{n\hbar^2}{2m_e^*}\left(\frac{\pi}{L_z}\right)^2 \quad (1)$$

Where m_e* is mass of the electron in the conduction band, in GaAs, $m_e = 0.067m_o$
L_Z is the length of the quantum well.
$\hbar$ is the Planck's constant =
ΔE is the transition energy between the 2 subbands and can be obtain or calculated using

$$E_{12} = E2 - E1 \quad (2)$$

Moreover, from (M. C. Wu, n.d.), along the dipole moment after the projection of a photon, the optical absorption coefficient can be derived as follows:
From Fermi's Golden Rule, which describes the transition rate between quantum states under a perturbation:

$$g(\Delta E) = \frac{1}{\pi}\frac{(\Gamma/2)}{\Delta E^2+(\Gamma/2)^2} \quad (3)$$

Here, H′H'H′ is the perturbation Hamiltonian due to the electromagnetic wave, and δ is the Dirac delta function enforcing energy conservation. For an electric dipole interaction, the perturbation is

$$g(\Delta E - \hbar\omega) = \frac{1}{\pi}\sum_{1\neq 2}\frac{(\Gamma|2)}{(\Delta E-\hbar\omega)^2+(\Gamma/2)^2} \quad (4)$$

Where $\vec{\mu}_{ba} = -e\langle b|\vec{r}|a\rangle$ is the transition dipole momentd $\vec{E}$is the electric field of the light. Therefore, the matrix element becomes:

$$g = \frac{1}{\pi}\frac{1}{(\Gamma/2)} \quad (5)$$

The **absorbed power per unit volume** is obtained by summing over all transitions and including the occupation probabilities of initial and final states:

$$\mu_{21} = e\int_0^{L_z}\psi_2(z)z\psi_{1(z)}\,dz \quad (6)$$

Substituting Transition Rate:

$$\psi_{1(z)} = \sqrt{\frac{2}{L_z}}\sin\left(\frac{\pi}{L_z}z\right) \quad (7)$$

Absorption Coefficient Definition:

$$\psi_{2(z)} = \sqrt{\frac{2}{L_z}}\sin\left(\frac{\pi}{L_z}z\right) \quad (8)$$

Substituting into Absorption Coefficient:

$$\mu_{21} = \frac{2e}{L_z}\int_0^{Lz} sin\left(\frac{2^{\pi}}{L_z}z\right) z\, sin\left(\frac{\pi}{L_z}z\right) dx \quad (9)$$

Replace Delta Function with Lorentzian:

$$\alpha(\hbar\omega) = {}^{2\pi}/_{n_r V c\epsilon_0}\sum g(E_b - E_a - \hbar\omega)|\hat{e}\cdot\vec{\mu}_{ba}|^2(f_b - f_a)$$

(10)

Where ω is the frequency of the Photon energy, n_r is the refractive index, C is the velocity of light, g $(E_b - E_a - \hbar\omega)$ is the line shape function, of electronic charge e with intersubband dipolemoment μ_a, V is the volume of entire material, ϵo permittivity of the material, f^b and f^a are the carrier densities populating subbands a and b, respectively.

Considering numerical calculation, calculated transition adjusted to a simple Lorentzian approximation will be given as

$$g(\Delta E) = \frac{1}{\pi}\frac{(\Gamma/2)}{\Delta E^2+(\Gamma/2)^2} \quad (11)$$

Where Γ is the line width.

Interms of photon energy the Modified Lorentzian approximation can be written as

$$g(\Delta E - \hbar\omega) = \frac{1}{\pi}\sum_{1\neq 2}\frac{(\Gamma|2)}{(\Delta E-\hbar\omega)^2+(\Gamma/2)^2} \quad (12)$$

Where ΔE and $\hbar\omega$ are the transition photons energy between subband and the adjusted frequency repectively.

However, transition occurs at the top conduction subbandcorsponds to the higestsubband, after the photon emission with electrons being annihilated from subband a= a to b = 2.

Therefore, setting (ΔE - $\hbar\omega$) = 0 one gets

$$g = \frac{1}{\pi}\frac{1}{(\Gamma/2)} \quad (13)$$

where Γ is the resulting Lorentzian broadening term, which we refer as dephasing energy in the subbands. Furthermore, the dipole moment is obtained by normalization of the enveloped wavefunction along the quantum well growth direction z, which is due to the electron excitation by the light

beam this can be expressed in the form

$$\mu_{21} = e\int_0^{L_z}\psi_2(z)z\psi_{1(z)}\,dz \quad (14)$$

Where

$$\psi_{1(z)} = \sqrt{\frac{2}{L_z}}\sin\left(\frac{\pi}{L_z}z\right) \quad (15)$$

And

$$\psi_{2(z)} = \sqrt{\frac{2}{L_z}}\sin\left(\frac{\pi}{L_z}z\right) \quad (16)$$

However, to solve for the intersubband dipole moment we substituted (14) and (15) into (16), we get

$$\mu_{21} = \frac{2e}{L_z}\int_0^{Lz} sin\left(\frac{2^{\pi}}{L_z}z\right) z\, sin\left(\frac{\pi}{L_z}z\right) dx \quad (17)$$

Integrating equations (9) simplifies to

$$\mu_{21} = -\frac{16}{9\pi^2}eL_z \quad (18)$$

Equation (18) is the resulting dipole moment of the quantum well. We will now analyze the absorption coefficient due to intersubband transition in quantum well of GaAs/AlGaAs. Equation (18) lead to the absorption related to absorption co efficient of the intersubband governed by

$$(\hbar w) = \frac{\pi\omega}{n_r c\epsilon_0}g(\Delta E - \hbar\omega)|\mu_{21}|^2(N2 - N_1) \quad (19)$$

Where N_1 and N_2 are the population densities of the first and second subbands respectively.

If N_2 = 0, in which $E_1 < E_F < E_2$ in subband 1, then we find

$$\alpha(\hbar w) = \frac{\pi\omega}{n_r c\epsilon_0}g(\Delta E - \hbar\omega)|\mu_{21}|^2 N_1 \quad (20)$$

Which is proportional to doping concentration. Moreover, with $E_2 < E_F$ in subband 2, then

$$N_1 = \frac{m_e^* k_B T}{\Pi\hbar^2 L_z}\ln\left[1 + e\left(\frac{E_F - E_1}{k_B T}\right)\right] \quad (21)$$

Where K_B is Boltzman's constant, T temperature and E_F is Fermi energy. Equation (21) can be simplified to

$$N_1 \approx \frac{m_e^*}{\pi\hbar^2 L_z}(E_F = -E_1) \quad (22)$$

And subsequently

$$N_2 \approx \frac{m_e^*}{\pi\hbar^2 L_z}(E_F = -E_2) \quad (23)$$

Finally, the optical absorption coefficient can be written as

$$\propto(\hbar\omega) = \frac{\Pi\omega}{n_r c\epsilon_0} g(\Delta E - \hbar\omega)\left(\frac{16}{9\Pi^2} e L_z\right)^2 \quad (24).$$

Which is independent of doping concentration. The peak absorption is obtained where ΔE= ħω and can be expressed as

$$\alpha_{max}(\hbar\omega) = \frac{\omega}{n_r c\epsilon_0}\frac{1}{(\Gamma/2)}\left(\frac{16}{9\Pi^2} e L_z\right)^2 N \cdot (25)$$

RESULTS AND DISCUSSION

The results were simulated using equation (24) within THZ spectrum region, with doping concertation N= 1 x10^{40}cm^{-3}. We plotted for QW width for 25nm, 30nm, 35nm and 40nm, Fig 1 to Fig 4, respectively all with dephasing energy of 8meV, 12meV, and 16meV.

we can clearly see a redshift in Fig 2 to Fig 4, which means increasing the QW width results in redshift of the absorbed edge. This is due to wider QW allows lower energy confinement states. The absorption peaks become more shaper as the QW widens, which is in agreement with (J. Zhang, H. Liu, 2021) and (Unuma et al., 2003)

The dephasing energy (Γ) accounts for broadening mechanisms such as phonon interactions, impurities, and other scattering processes. Higher Γ lead to a broader absorption with less peaks, indicating increased scattering and reduced coherence of electronic state as we can see from all the figures. Lower Γ (8meV results in shaper peaks, which is in agreement with(Adamu et al., 2019), (L. Zhang, Y. Chen, 2022) and(L. Zhang, Y. Chen, 2022)

In summary, the results highlight that both the quantum well width and dephasing energy significantly influence the optical absorption characteristics. Precise control over these parameters is vital for optimizing the performance of quantum well-based optoelectronic devices. For future work, such transmissions, how Doping concentration effect Absorptions and other optical parameters.

Overall, the simulation results align with published experimental data and demonstrate the effectiveness of theoretical mod0eling in guiding the development of QW-based optoelectronic devices.

.

Table 1: List of parameters used in the calculations.

Parameter	Value
$\hbar$	1.054 x 10-34 (Js)
m^*	0.067 m_o (Kg)
m_o	9.109 x 10-31 (Kg)
e	1.602 x 10-19 (C)
K_B	1.381 x 10-23 (J/K)
ϵ_0	8.854 x 10-12 (F/m)
T	300(K)
C	300000000 (m/s)

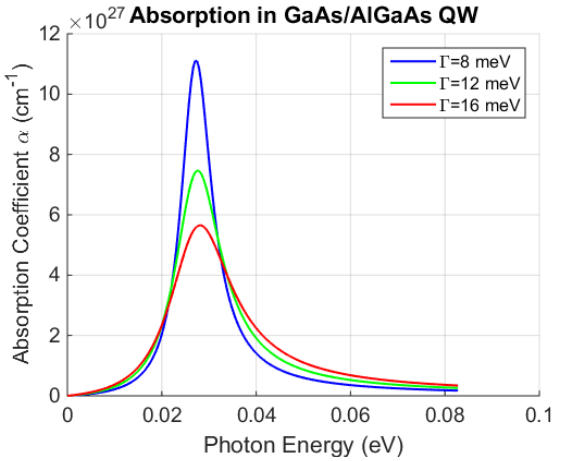

Fig1: Absorption against photon energy with width of the QW Lz =25nm.

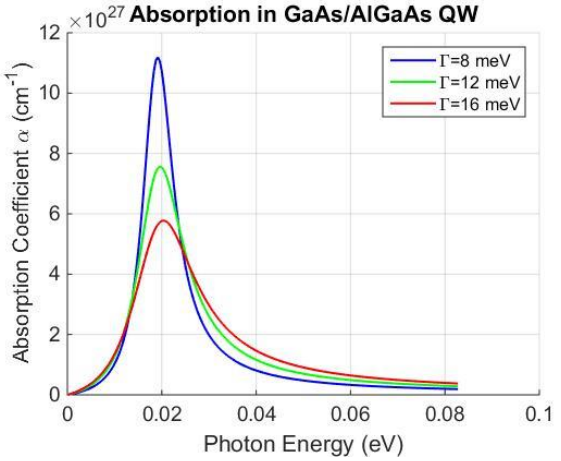

Fig 2: Absorption against photon energy with width of the QW Lz =30nm.

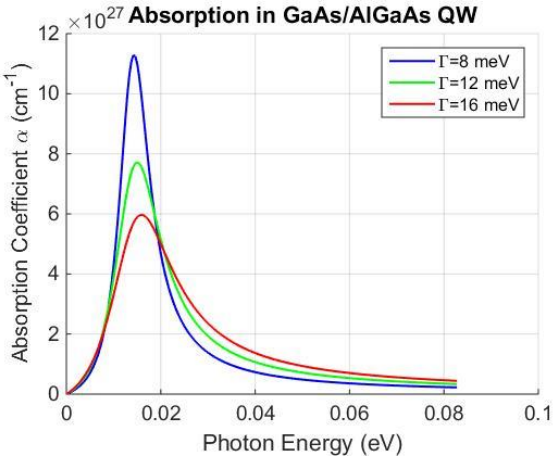

Fig 3: Absorption against photon energy with width of the QW Lz =35nm.

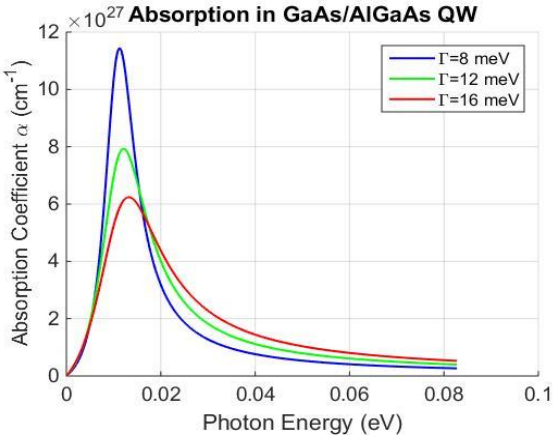

Fig 4: Absorption against photon energy with width of the QW Lz =40nm.

CONCLUSION

In this work, the optical absorption properties of GaAs/AlGaAs quantum wells were simulated and analyzed with respect to quantum well width and dephasing energy.

Accurate modeling of quantum well absorption spectra require considering both well width and dephasing energy. The well width determines the energy position and the nature of the absorption features, while dephasing influences their shape and sharpness. These parameters are crucial for designing optoelectronic devices, such as lasers and detectors, where spectral selectivity and coherence are essential.

Understanding how the well width affects the energy levels allows engineers to tailor devices for specific wavelength operation. Managing dephasing mechanisms (e.g., through material quality improvements) can enhance device performance by sharpening spectral features and increasing efficiency.

REFERENCE

Adamu, S. B., Adamu, S. B., Faragai, I. A., & Ibrahim, U. (2019). *Optical Absorption in GaAs/AlGaAs Quantum Well due to Intersubband transitions*.

Albo A., Fekete, D., & Bahir, G. (2012). Electronic bound states in the continuum above (Ga,In)(As,N)/(Al,Ga)As quantum wells. *Physical Review B - Condensed Matter and Materials Physics*, *85*(11). https://doi.org/10.1103/PhysRevB.85.115307

J. Zhang, H. Liu, and X. W. (2021). Effects of Quantum Well Width and Temperature on the Optical Absorption Spectra of GaAs/AlGaAs Quantum Wells. *Materials*, *14*(19), 2345.

Jr, M. F. P., &Faragai, I. A. (2014). *Coupling of THz radiation with intervalence band transitions in microcavities*. *22*(3), 3439–3446. https://doi.org/10.1364/OE.22.003439

L. Zhang, Y. Chen, and M. W. (2022). Dephasing mechanismsin semiconductor quantum wells: A review of experimental and theoretical advances. *Journal of Applied Physics*, *131*(12), 12090.

Liu, S., Han, Q., Luo, W., Lei, W., Zhao, J., Wang, J., Jiang, Y., & Raschke, M. B. (2024). Recent progress of innovative infrared avalanche photodetectors. *Infrared Physics & Technology*, 105114. https://doi.org/10.1016/j.infrared.2023.105114

Pereira, M. F., & Faragai, I. A. (2013). *THz Intervalence Band Polaritons and Antipolaritons*. 13–15.

Redaelli, L., Mukhtarova, A., Ajay, A., Núñez-Cascajero, A., Valdueza-Felip, S., Bleuse, J., Durand, C., Eymery, J., & Monroy, E. (2015). Effect of the barrier thickness on the performance of multiple-quantum-well InGaN photovoltaic cells. *Japanese Journal of Applied Physics*, *54*(7). https://doi.org/10.7567/JJAP.54.072302

Unuma, T., Yoshita, M., Noda, T., Sakaki, H., & Akiyama, H. (2003). Intersubband absorption linewidth in GaAs quantum wells due to scattering by interface roughness, phonons, alloy disorder, and impurities. *Journal of Applied Physics*, *93*(3), 1586–1597. https://doi.org/10.1063/1.1535733

Wu, C. H., Ku, C. J., Yu, M. W., Yang, J. H., Wu, P. Y., Huang, C. Bin, Lu, T. C., Huang, J. S., Ishii, S., & Chen,

K. P. (2023). Near-Field Photodetection in Direction Tunable Surface Plasmon Polaritons Waveguides Embedded with Graphene. *Advanced Science*, *10*(30). https://doi.org/10.1002/advs.202302707

Wu, M. C. (n.d.). *EE 232 Lightwave Devices Lecture 9: Intersubband Absorption i Q t W ll in Quantum Wells*.

Zhang, G., Xu, C., Sun, D., Wang, Q., Lu, G., & Gong, Q. (2024). Metasurface-tuned light-matter interactions for high-performance photodetectors. *Fundamental Research*. https://doi.org/10.1016/j.fmre.2024.01.002