



Advancements in Quantum Well Structures: Exploring V-shaped Double Quantum Wells

Summer Research Project

By

Ayush Mohapatra

1st year Integrated M.Sc.

National Institute of Science Education and Research

(NISER), Bhubaneswar- 752050

Roll No: 2311047

Batch: 2023

Supervisor:

Dr. Satchidananda Rath

Associate Professor of Physics

School of Basic Sciences

Indian Institute of Technology, Bhubaneswar- 752050

srath@iitbbs.ac.in

DECLARATION

I, Ayush Mohapatra, hereby declare that the internship report titled “Advancements in Quantum Well Structures: Exploring V-shaped Double Quantum Wells” is a record of my own work and the experiences gained during my summer internship, carried out under the guidance of Dr. Satchidananda Rath during my summer internship at IIT Bhubaneswar.

Date - 31/07/2024

Ayush Mohapatra

Place – Bhubaneswar

NISER, Bhubaneswar



CERTIFICATE



This is to certify that Mr. Ayush Mohapatra, a student of NISER (National Institute of Science Education and Research), Bhubaneswar has successfully completed Training from 16 June 2024 to 31 July 2024 at IIT (Indian Institute of Technology), Bhubaneswar and has made the Training project report under my guidance.

Dr. Satchidananda Rath

Associate Professor of Physics

School of Basic Sciences

Indian Institute of Technology, Bhubaneswar

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Ayush Mohapatra

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List of Abbreviations

- **VDQW** - V-shaped Double Quantum Well
- **QW** - Quantum Well
- **Al_xGa_{1-x}As** - Aluminium Gallium Arsenide (used as an example material for quantum wells)
- **F_{ext}** - External Electric Field
- **meV** - Milli Electron Volts
- **Å** - Angstrom
- **CMOS** - Complementary Metal-Oxide-Semiconductor
- **QD** - Quantum Dot
- **LED** - Light Emitting Diode
- **2DEG** - Two-Dimensional Electron Gas
- **Ψ(z)** - Wave Function as a function of position z
- **N_d** - Doping Concentration

Abstract

This study investigates the electronic properties of a V-shaped double quantum well (VDQW) structure composed of $\text{Al}_x\text{Ga}_{1-x}\text{As}$. The VDQW potential is realized by altering the conduction band edge of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ through a linear variation of the alloy fraction x within the wells. By solving the coupled Schrödinger and Poisson equations, we obtain the subband energy levels E_j and wave functions $\psi_j(z)$. The results reveal that the V-shaped confinement potential significantly influences the electronic states, with the presence of asymmetric doping concentrations and external electric fields further modifying the potential profile and electron distribution. Our findings demonstrate that the energy levels and wave functions exhibit expected quantized behaviour, providing valuable insights into the design and optimization of quantum well structures for electronic and optoelectronic applications. The study underscores the importance of theoretical modelling in predicting the behaviour of complex semiconductor heterostructures, contributing to advancements in semiconductor technology.

Introduction

In recent years, there has been a significant surge of interest in the study of semiconductor quantum well (QW) structures due to their diverse confinement potentials. These structures come in various shapes, including square, parabolic, graded, V-shaped, inverse parabolic, and triangular, among others, each offering unique advantages for device applications. The potential profile of a quantum well has a direct impact on the subband energy states, making it possible to manipulate the electronic properties of two-dimensional electron gas (2DEG) systems by varying the confinement potential.

Nitride-based V-shaped InGaN/GaN quantum wells (QWs) are a prominent example, used to develop blue light-emitting diodes (LEDs). These V-shaped QWs exhibit higher intensity and narrower linewidths compared to conventional rectangular QWs, making them more efficient for optical applications. Similarly, triangular InGaN/GaN QWs demonstrate higher electron-hole wave function overlap, leading to increased optical gain and efficiency. Parabolic QW structures have also been proposed for high-efficiency light emitters in both light-emitting diodes and laser diodes, due to their ability to concentrate carriers in the active region.

A double quantum well (DQW) system is particularly intriguing due to its combination of tunneling coupling and confinement effects. This system features the coupling of subband wave functions from individual wells, causing the splitting of energy levels. By adjusting structural parameters such as well width, barrier width, and doping concentration, the strength of this coupling can be tuned, significantly affecting the subband wave functions and energy levels.

In the symmetric state, the ground subband energy level (E_0) and the first excited energy level (E_1) form a doublet, with their wave functions (ψ_0 and ψ_1) spreading across both wells. This symmetry and antisymmetry of wave functions play a critical role in the behaviour of the system. Furthermore, near resonance, the energy levels E_0 and E_1 exhibit anticrossing, a phenomenon where the levels repel each other as they come close to intersecting.

Research has shown that an asymmetric DQW system can exhibit resistance resonance, characterized by a peak in electrical resistance near the resonance of subband states between the wells as a function of the external electric field. This effect underscores the

intricate interplay between structure, potential profile, and external fields in determining the electronic properties of quantum well systems.

Theory

We consider a V-shaped double quantum well (VDQW) structure made of $Al_xGa_{1-x}As$ as shown in Figure 1(a). The VDQW potential is realised by altering the conduction band edge of $Al_xGa_{1-x}As$, by varying the alloy fraction x linearly within the wells, i.e. $x = 0$ at the centre to $x = x_w (\leq 0.3)$ at the edges of the wells and $x = 0.3$ for the barriers.

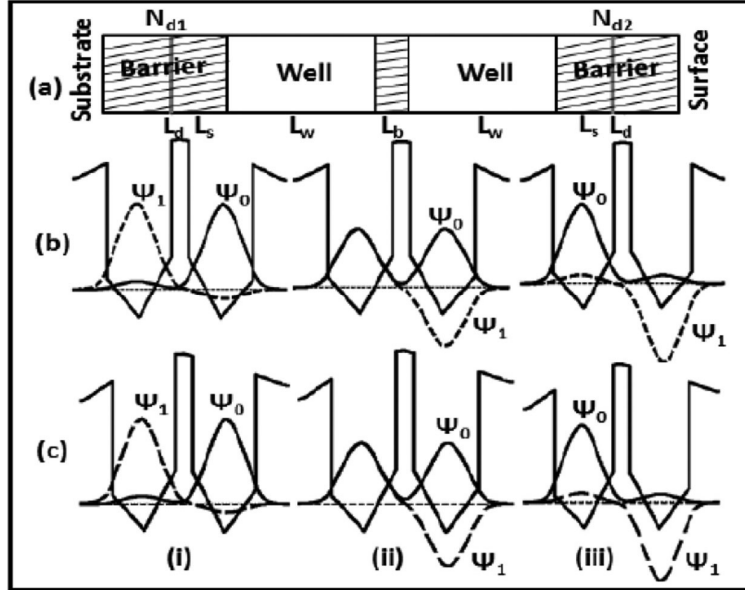


Figure 1. (a): Schematic structure layout of $Al_xGa_{1-x}As$ based V-shaped double quantum well (VDQW) structure of well width L_w (Å), central barrier width L_b (Å), spacer width L_s (Å) and Sidelta-doped layers of width L_d (Å), (b): Simulated results of the potential profile $V_{eff}(z)$ with subband energy levels E_0 and E_1 (meV) and wave functions ψ_0 and ψ_1 for $L_d = 20$ Å, $L_s = 60$ Å, $L_w = 150$ Å, $L_b = 40$ Å, $x_w = 0.1$ and $(N_{d1}, N_{d2}) = (1, 1) \times 10^{18} \text{ cm}^{-3}$ taking (i) $F_{ext} = -0.5$ kV/cm, (ii) $F_{ext} = 0$ kV/cm and (iii) $F_{ext} = 0.5$ kV/cm. Fig.1(c): The same plots for the asymmetrically doping concentrations $(N_{d1}, N_{d2}) = (1.5, 0.5) \times 10^{18} \text{ cm}^{-3}$ for (i) $F_{ext} = -5.3$ kV/cm, (ii) $F_{ext} = -4.8$ kV/cm and (iii) $F_{ext} = -4.3$ kV/cm.

The V-shaped confinement structure potential for the electrons is given by:

$$V_S(z) = \begin{cases} V_w \left| \frac{|z| - (L_b + L_w)/2}{(L_w/2)} \right| & (L_b/2) < |z| < (L_b/2) + L_w \\ V_b & \text{otherwise} \end{cases} \quad (1)$$

Here V_b , and V_w are the heights of the barrier, and V-shaped potentials at the edges of the wells respectively. These are calculated using the relation, $V(x) = 0.693x + 0.222x^2$ eV. The structure parameters L_b , and L_w are the central barrier width, and well width respectively. The delta doping layers of thickness L_d lie in the outer barriers at a spacer distance L_s from the interfaces with doping concentration N_{d1} towards the substrate while N_{d2} towards the surface. The difference in N_{d1} and N_{d2} leads to the asymmetric potential structure. The doping concentration distribution is given by:

$$N_D(z) = \begin{cases} N_{d1} & -(L_d + L_s + L_w + L_b/2) < z < -(L_s + L_w + L_b/2) \\ N_{d2} & (L_b/2 + L_w + L_s) < z < (L_b/2 + L_w + L_s + L_d) \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

Within effective mass approximation, the subband energy levels E_j , and wave functions $\psi_j(z)$ of the two-dimensional electron gas (2DEG) along growth direction (z-axis) are given by:

$$\psi_{j\vec{k}}(\vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}}}{\sqrt{A}} \psi_j(z) \quad (3)$$

$$E_{j\vec{k}} = E_j + \frac{\hbar^2 k^2}{2m^*} \quad (4)$$

where $\vec{r}$ is the position vector, and $\vec{k}$ is the wave vector parallel to the interface plane.

A , m^* and j are the sample area, electron effective mass and subband index respectively.

The wave functions $\psi_j(z)$, and energy levels E_j satisfy the Schrödinger equation:

$$\left[\frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} + V_{eff}(z) \right] \psi_j(z) = E_j \psi_j(z), \quad (5)$$

The potential $V_{eff}(z) = V_H(z) + V_S(z) + V_F(z)$. $V_S(z)$ is the confinement potential due to the V-shaped structure as given in Eq.1. $V_F(z)$ is the potential due to the applied electric field F_{ext} along the growth direction, i.e. $V_F(z) = eF_{ext}z$, and $V_H(z)$ is the Hartree potential governed by the Poisson's equation:

$$\frac{d^2 V_H}{dz^2} = \frac{4\pi e^2}{\epsilon_0} [N_D(z) - n_e(z)]. \quad (6)$$

The doping concentration distribution $N_D(z)$ is expressed in Eq.2, and the electron distribution $n_e(z)$ is given as:

$$n_e(z) = \sum_j n_j |\psi_j(z)|^2 \quad -\infty < z < +\infty, \quad (7)$$

The sum over j represents the subband levels. n_j is the areal electron density of the j^{th} subband which relates to the Fermi energy E_F as:

$$n_j = \left(\frac{m^* k_B T}{\pi \hbar^2} \right) \ln [1 + e^{(E_F - E_j)/k_B T}] \quad (8)$$

The 2DEG density $N_s = \sum_j^N n_j$. At $T=0$ K, N_s can be written as:

$$N_s = \frac{m^*}{\pi \hbar^2} \sum_{j=1}^N (E_F - E_j) \theta(E_F - E_j) \quad (9)$$

where N is the number of filled levels and θ is the Heaviside step function. The Fermi energy E_F also relates to the charge neutrality condition throughout the system:

$$\int_{-\infty}^{\infty} \left(\sum_j n_j |\psi_j(z)|^2 - N_D^+(z) \right) dz = 0. \quad (10)$$

We assume that the source of the carriers arises from the delta doping layers in the side barriers (Eq. 2) only, and at $T=0$ K all the donors are ionised. The Fermi level E_F is calculated using the above Eqs.8–10.

The wave functions $\psi_j(z)$, and energy levels E_j are obtained by solving one-dimensional Schrodinger equation, and Poisson's equation. We solve Poisson's equation using the variational method to obtain an analytical expression for $V_{eff}(z)$. Then we adopt multistep approximation for the potential $V_{eff}(z)$ to obtain the transmission coefficient T across $V_{eff}(z)$ to calculate E_j and $\psi_j(z)$ numerically. In the multistep approximation, $V_{eff}(z)$ and the electron effective mass $m^*(z)$ are varied as multistep functions along the growth direction i.e. z -axis. The potential $V_{eff}(z)$ is divided into segments, say, $j = 1, 2, \dots, N$. In each segment j , the potential is assumed to be constant (V_j), i.e. equal to the average of the potential energy of the two ends of that strip. By increasing the number of strips N , the multi-step potential $V_{eff}(z_j)$ reduces to the continuous potential $V_{eff}(z)$. The continuity of $\psi_j(z)$ and $(1/m^*(z)) (d\psi_j(z)/dz)$ at each boundary leads to obtain an expression for T across $V_{eff}(z_j)$.

The maxima of the transmission probability T occur as the electron energy E becomes equal to the discrete allowed energy levels in the well, i.e. $E = E_j$. By varying the input energy E from 0 to V_b , T^{-1} is computed across $V_{eff}(z_j)$ to obtain $E_j(z)$ and $\psi_j(z)$. Our procedure is repeated several times, until we obtain the consistent results of $E_j(z)$ and $\psi_j(z)$ within a difference of 0.01%.

In [Figure 1\(b\)](#), we present the $V_{eff}(z)$, E_j , and $\psi_j(z)$ of the VDQW for $L_d = 20 \text{ \AA}$, $L_s = 60 \text{ \AA}$, $L_w = 150 \text{ \AA}$, $L_b = 40 \text{ \AA}$, $x_w = 0.1$, and $(N_{d1}, N_{d2}) = (1, 1) \times 10^{18} \text{ cm}^{-3}$ taking $F_{ext} = -0.5, 0.0$, and 0.5 kV/cm . For $F_{ext} = 0 \text{ kV/cm}$, the VDQW potential is symmetric about the central barrier. The wave functions $\psi_0(z)$, and $\psi_1(z)$ extend into both the well equally in symmetric and anti-symmetric manner respectively exhibiting resonance. A slight change in F_{ext} , in either side, i.e. $F_{ext} = \pm 0.5 \text{ kV/cm}$, the system becomes asymmetric, and resonance is lost. For $F_{ext} = -0.5 \text{ kV/cm}$, $\psi_0(z)$ and $\psi_1(z)$ almost lie in the wells towards the surface and the substrate respectively. For $F_{ext} = 0.5 \text{ kV/cm}$ vice versa occurs. In [Figure 1\(c\)](#), we consider unequal doping concentrations, $(N_{d1}, N_{d2}) = (1.5, 0.5) \times 10^{18} \text{ cm}^{-3}$ so that at $F_{ext} = 0 \text{ kV/cm}$ the system is asymmetry. The asymmetry in potential due to doping concentrations is compensated through the application of F_{ext} . As a result, the resonance of subband states is achieved at $F_{ext} = -4.8 \text{ kV/cm}$. Consequently, the wave function $\psi_0(z)/\psi_1(z)$ equally extends symmetrically/anti-symmetrically into both the wells of the VDQW. Whereas, for other field values, $F_{ext} = -5.3 \text{ kV/cm}$, and $F_{ext} = -4.3 \text{ kV/cm}$, $\psi_0(z)$, and $\psi_1(z)$ are unequally distributed in the wells, similar to that presented in [Figure 1\(b\)](#).

Methodology

In this study, we aim to solve the Schrödinger and Poisson equations for a V-shaped double quantum well (VDQW) structure to obtain the electron subband energy levels and corresponding wave functions. The methodology includes the following:

Parameters

The parameters used in the study of the V-shaped double quantum well (VDQW) structure are as follows:

- **Material Composition:** The VDQW is made of $\text{Al}_x\text{Ga}_{1-x}\text{As}$.
- **Structural Dimensions:**
 - **L_d:** Delta doping layer thickness, 20 Å
 - **L_s:** Spacer distance, 60 Å
 - **L_w:** Well width, 150 Å
 - **L_b:** Barrier width, 60 Å
- **Doping Concentration:**
 - **N_{d1}:** Doping concentration towards the substrate, $1.0 \times 10^{18} \text{ cm}^{-3}$
 - **N_{d2}:** Doping concentration towards the surface, $1.0 \times 10^{18} \text{ cm}^{-3}$
- **Effective Mass:** $m^* = 0.067 \times 9.10938356 \times 10^{-31} \text{ kg}$
- **External Electric Field:** $F_{\text{ext}} = -0.5 \text{ kV/cm}$
- **Grid for Z Axis:**
 - **Z_{min}:** -480 Å

- Z_{max} : 480 Å
- Z_{points} : 1000 points

These parameters define the physical and structural characteristics of the VDQW system, influencing the potential profile, energy levels, wave functions, and current density calculations.

Numerical Solution

- 1) Define the doping concentration and initial electron density.
- 2) Solve Poisson's equation to obtain the Hartree potential $V_H(z)$.
- 3) Define the total effective potential $V_{\text{eff}}(z)$.
- 4) Discretize the Hamiltonian and solve the eigenvalue problem to obtain energy levels and wave functions.
- 5) Apply Gaussian broadening to the calculated wave functions to account for tunneling effects and enhance the visibility of the wave functions.

Code Implementation

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.constants import hbar, e, epsilon_0
from scipy.linalg import eigh

# Constants
m_star = 0.067 * 9.10938356e-31 # Effective mass
in kg (for GaAs)
hbar = 1.0545718e-34 # Reduced Planck constant in
J-s
eV_to_J = 1.60218e-19 # Conversion from eV to J
Angstrom_to_meter = 1e-10 # Conversion from Å to
m
kV_per_cm_to_V_per_m = 1e5 # Conversion from
kV/cm to V/m
# Given parameters in Ångströms
L_d = 20 # Å
L_s = 60 # Å
L_w = 150 # Å
L_b = 60 # Å
N_d1 = 1.0e18 * 1e6 # cm^-3 to m^-3 equivalent
N_d2 = 1.0e18 * 1e6 # cm^-3 to m^-3 equivalent
F_ext = -0.5 * kV_per_cm_to_V_per_m # External
electric field in V/m
# Grid for z in Ångströms
z_min = -2 * (L_d + L_s + L_w + L_b / 2)
z_max = 2 * (L_d + L_s + L_w + L_b / 2)
z_points = 1000
z = np.linspace(z_min, z_max, z_points)
dz = z[1] - z[0]
# Define the doping concentration distribution
N_D(z)
def N_D(z):
    if -(L_d + L_s + L_w + L_b / 2) < z < -(L_s + L_w +
L_b / 2):
        return N_d1
    elif (L_b / 2 + L_w + L_s) < z < (L_b / 2 + L_w + L_s
+ L_d):
        return N_d2
    else:
        return 0
N_D_values = np.array([N_D(zi) for zi in z])
# Initial guess for n_e(z) (can be zeros initially)
n_e_values = np.zeros_like(z)
```

```
# Solve Poisson's equation using finite difference
method
def solve_poisson(N_D_values, n_e_values, dz,
z_points):
    V_H = np.zeros(z_points)
    for _ in range(1000): # Iterate to solve Poisson's
equation
        V_H[1:-1] = 0.5 * (V_H[:-2] + V_H[2:] - dz**2 *
(4 * np.pi * e / epsilon_0) * (N_D_values[1:-1] -
n_e_values[1:-1]))
    return V_H
V_H_values = solve_poisson(N_D_values,
n_e_values, dz * Angstrom_to_meter, z_points)
# Define the confinement potential V_S(z)
def V_S(z):
    if -30 < z < 30:
        return 280
    elif 30 < np.abs(z) < 180:
        return 250 * np.abs((np.abs(z) - 105) / 75)
    elif -240 < z < -180:
        return 0.366667 * (z + 240) + 228
    elif 180 < z < 240:
        return -0.366667 * (z - 180) + 250
    else:
        return 228
V_S_values = np.array([V_S(zi) for zi in z])
# Potential due to the external electric field V_F(z) = e
F_ext z
V_F_values = e * F_ext * z * Angstrom_to_meter #
Convert z from Å to meters
# Total effective potential V_eff(z)
V_eff_values = V_H_values + V_S_values +
V_F_values / eV_to_J # Correct units conversion
# Discretize the Hamiltonian
Hamiltonian = np.zeros((z_points, z_points))
for i in range(1, z_points - 1):
    Hamiltonian[i, i] = -2.0
    Hamiltonian[i, i - 1] = 1.0
    Hamiltonian[i, i + 1] = 1.0
Hamiltonian *= -hbar**2 / (2 * m_star * (dz *
Angstrom_to_meter)**2)
```

```

# Add the potential to the Hamiltonian
for i in range(z_points):
    Hamiltonian[i, i] += V_eff_values[i] * eV_to_J # Convert eV to J
# Solve the eigenvalue problem
eigenvalues, eigenvectors = eigh(Hamiltonian)
# Convert the eigenvalues from Joules to eV
eigenvalues = eigenvalues / eV_to_J
# Define occupation numbers (example, can be adjusted as needed)
n_j = np.ones(len(eigenvalues)) # Example: each state is equally occupied
# Calculate electron density n_e(z)
n_e_values = np.sum([n_j[j] * np.abs(eigenvectors[:, j])**2 for j in
range(len(eigenvalues))], axis=0)
# Define Gaussian broadening function
def gaussian_broadening(psi, sigma):
    broadened_psi = np.zeros_like(psi)
    for i in range(len(psi)):
        broadened_psi += psi[i] * np.exp(-0.5 * ((z - z[i]) / sigma)**2)
    return broadened_psi
# Apply Gaussian broadening to wave functions
sigma = 25 # Broadening factor in Å
broadened_wave_functions = [gaussian_broadening(eigenvectors[:, i], sigma)
for i in range(4)] # Include first four wave functions
# Plot the potential profile and the first few wave functions
plt.figure(figsize=(10, 6))
plt.plot(z, V_eff_values, label='Potential Profile $V(z)$ (meV)', color='red')
scaling_factor = 60 # Adjust scaling factor for visibility
linewidth = 3 # Increase linewidth for wave functions
offsets = [24, 24, 36, 36] # Offsets for the wave functions
for i in range(4): # Plot the first four wave functions
    plt.plot(z, broadened_wave_functions[i] * scaling_factor + offsets[i],
label=f'$\psi_{i+1}(z)$', E{i+1} = {eigenvalues[i+1]:.2f} eV', linewidth=linewidth)
plt.xlabel('z (Å)')
plt.ylabel('Potential Profile V(z) and Wave functions $\psi(z)$')
plt.title('Broadened Wave functions $\psi_0(z)$ to $\psi_3(z)$ with $V(z)$')
plt.legend()
plt.xlim(-350, 350) # Zoom in on the region of interest
plt.ylim(-150, 350) # Adjust the y-axis limits for better visibility
plt.grid(True)
plt.show()
# Print the energy levels
for i in range(4):
    print(f'$E_{i+1} = {eigenvalues[i+1]:.2f}$ eV')

```

Results

The analysis of the V-shaped double quantum well (VDQW) structure yields the following results:

1. Potential Profile:

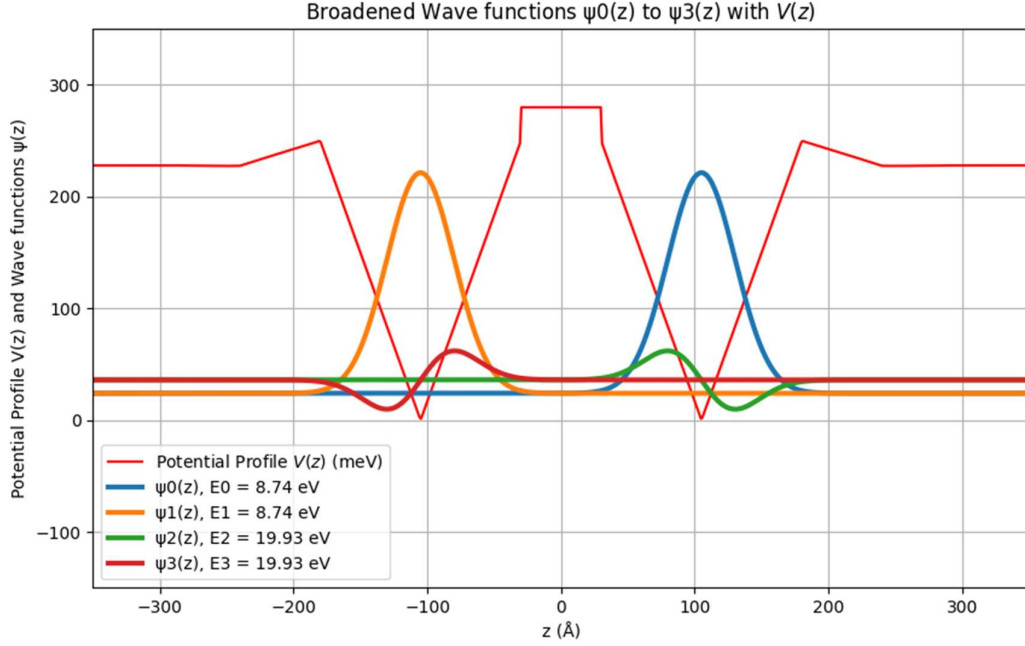
- The effective potential $V_{\text{eff}}(z)$ is obtained by combining the Hartree potential $V_H(z)$, the V-shaped confinement potential $V_S(z)$, and the potential due to the external electric field $V_F(z)$.
- The potential profile exhibits distinct features corresponding to the structural parameters and doping concentrations.

2. Energy Levels:

- The subband energy levels E_j are determined by solving the Schrödinger equation.
- The lowest four energy levels E_0 , E_1 , E_2 and E_3 are found to be 8.74 eV, 8.74 eV, 19.93 eV and 19.93 eV, respectively.

3. Wave Functions:

- The corresponding wave functions $\psi_0(z)$, $\psi_1(z)$, $\psi_2(z)$ and $\psi_3(z)$ are plotted.
- These wave functions are scaled for visibility and show expected symmetric and asymmetric behaviour within the wells.



These results illustrate the influence of the structural parameters and external electric field on the electronic properties of the VDQW system, providing insights into the behaviour of electrons in such confined potentials.

Conclusion

In this study, we investigated the electronic properties of a V-shaped double quantum well (VDQW) structure made of $\text{Al}_x\text{Ga}_{1-x}\text{As}$. By solving the Schrödinger and Poisson equations, we determined the effective potential profile $V_{\text{eff}}(z)$, subband energy levels E_j , and corresponding wave functions $\psi_j(z)$. The results reveal that the V-shaped confinement potential significantly influences the subband energy levels and the spatial distribution of wave functions, with asymmetries introduced by varying doping concentrations and external electric fields altering the potential profile and wave function localization. The calculated energy levels and wave functions exhibit expected behaviour, providing critical insights into the quantized nature of electron states in the

VDQW structure. The study also demonstrates the tunability of the VDQW system through external electric fields, which is essential for potential applications in electronic and optoelectronic devices. Overall, this research highlights the importance of theoretical modelling in predicting and optimizing the behaviour of complex quantum well structures, contributing to the advancement of semiconductor technology.

Keywords

double quantum wells, non-square quantum wells, V-shaped quantum well structure, optoelectronic Devices, energy Band Structure

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