# Theoretical Calculations of Wave Function and Absorption Coefficient for a InGaP/AlGaAs/GaAs Multiquantum Well Infrared Photodetector Structure

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#### Abstract

The theoretical calculation of wave function and the absorption coefficient are calculated for a new structure, which consists of  $n^+GaAs/In_{0.49}Ga_{0.51}P$  quantum well embedded in a GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As superlattice structure. The structure is designed for long wavelength infrared (8-12 µm) radiation detection. The transfer matrix method is used to solve Schroedinger equation for the wave function and the energy levels. The oscillator strength is determined for the calculation of the absorption coefficient. With the dimensions of 53 Å/40 Å  $n^+GaAs/In_{0.49}Ga_{0.51}P$  and 60 Å/40 Å GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As superlattice, respectively, the absorption coefficient for 8.3 µm detection at different temperature is illustrated. The energy levels and the wave function for the embedded well structure are also shown.

## 1. Introduction

Long wavelength infrared photodetectors (8-12 µm) are used in several applications, such as medical images, satellite surveillance, and target designators. From the relationship  $E(eV.) = \frac{1.24}{\lambda(\mu m)}$ , the transition energy for the long wavelength infrared is too small to rely on the transition between energy levels in bulk semiconductor material. Hence, researchers have been investigating different compound semiconductor materials and different structures to obtain the most efficient detectors. Intersubband transition in GaAs/AlGaAs multiquantum well was first observed by West and Eglash to indicate the optical absorption for long wavelength infrared radiation [1].

Beside the intersubband transition, the bound-to-miniband transition is investigated.

Several studies have demon-strated that improvement in optical absorption could be achieved through the bound-to-miniband transition in the multiquantum well and superlattice structure [2-4]. Here, the energy levels, oscillator strength, and the absorption coefficient of a n<sup>+</sup>GaAs/In<sub>0.49</sub>Ga<sub>0.51</sub>P quantum well embedded in a GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As superlattice structure, shown in Fig. 1 are calculated. The superlattice structure replaced a bulk-barrier region to ensure a miniband formation for the bound-to-miniband transition. The advantages of a superlattice barrier over a bulk barrier are the elimination of deep level recombination between single and double heterojunction [5] and the enhancement of the intersubband absorption [6].

To ensure the bound-to-miniband transition, the structure is designed such that the first energy level lies inside the  $n^+GaAs$  well and the excited energy level lies within the

miniband. The physical parameters of the structure are 53 Å n<sup>+</sup>GaAs (L<sub>w</sub>), 40 Å InGaP (L<sub>bw</sub>), 60 Å GaAs (L<sub>wsl</sub>), and 40 Å AlGaAs (L<sub>bsl</sub>). Energy levels can be obtained by solving the Schroedinger equation through the transfer matrix method.



Figure 1 a) Conduction band profile of the embedded well structure b) Bound-to-miniband transition.

#### 2. Theoretical Calculation

Energy levels in a quantum well structure can be determined by solving the Schroedinger equation for the wave function. The time-independent Schroedinger equation is written as [7]:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x) + v(x)\Psi(x) = -|E|\Psi(x)$$
(1)

The transfer matrix method is used in calculating the bound energies and wave function by simple multiplication of a 2-by-2 matrix [8]. To solve the wave function of an arbitrary structure, the wave function of each region is calculated. The general equation of the wave function for a region (j) is in the form of [7]:

$$\Psi(x) = A_j \exp\left[\kappa_j \left(x - x_{j-1}\right)\right] + B_j \exp\left[-\kappa_j \left(x - x_{j-1}\right)\right]$$
(2)  
where  $\kappa_j = i\sqrt{\frac{2m}{\hbar^2} \left(E - v_j\right)}$ 

The transfer matrix method is based on matching the wave function and its derivatives at the boundaries [9]. The value of the wave function must be equal at the boundaries and the value of the derivative is inversely proportional to the effective mass as shown [10]:

$$\Psi_{j}(\boldsymbol{x}_{j}) = \Psi_{j+1}(\boldsymbol{x}_{j+1})$$
(3)

$$\frac{1}{\mathbf{m}_{j}^{*}}\frac{\partial}{\partial \mathbf{x}}\left[\Psi_{j}\left(\mathbf{x}_{j}\right)\right] = \frac{1}{\mathbf{m}_{j+1}^{*}}\frac{\partial}{\partial \mathbf{x}}\left[\Psi_{j+1}\left(\mathbf{x}_{j+1}\right)\right] \quad (4)$$

From the wave function equation and the above conditions,  $A_{j+1}$  and  $B_{j+1}$  can be presented in term of  $A_j$  and  $B_j$  in a matrix form, which referred to as a 2 by 2 matrix ( $M_j$ ). Hence, for N number of regions, the matrix becomes:

$$\begin{bmatrix} \mathbf{A}_{\mathbf{N}-1} \\ \mathbf{B}_{\mathbf{N}-1} \end{bmatrix} = \mathbf{M}_{\mathbf{N}-2} \cdot \mathbf{M}_{\mathbf{N}-3} \cdot \dots \cdot \mathbf{M}_{1} \cdot \mathbf{M}_{0} \cdot \begin{bmatrix} \mathbf{A}_{0} \\ \mathbf{B}_{0} \end{bmatrix}$$
(5)

The allowed energy can be determined by setting the determinant of total matrix M to zero. The wave function coefficient is then calculated using the normalization condition, which is:

$$\int_{-\infty}^{\infty} \Psi \Psi^* dx = 1$$
 (6)

The absorption coefficient ( $\alpha$ ) is calculated from [11]:

$$\alpha(\hbar\omega) = \frac{\pi q^2 \hbar c \mu_0}{2m^* n_r} f_{nn} \cdot J_{nn} \cdot \Delta N \quad (8)$$

where

$$J_{mn} = \frac{2}{\pi} \frac{\hbar}{10^{-12}} \frac{1}{(E_{g} - \hbar\omega)^{2} + (\frac{\hbar}{10^{-12}})^{2}} \quad (9)$$
$$\Delta N = \frac{4\pi m^{*}}{h^{2}L} kT \ln \frac{1 + \exp\left(\frac{(E_{1} - E_{f})}{kT}\right)}{1 + \exp\left(\frac{(E_{2} - E_{f})}{kT}\right)} \quad (10)$$

$$E_{f} = \frac{kT}{q} \ln(e^{N_{d}/n_{0}} - 1)$$
(11)

$$n_{0} = \frac{m^{*}kT}{\pi\hbar^{2}L_{w}}$$
(12)

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 $J_{nn}$  is the joint density of state,  $\Delta N$  is the population difference of initial and final state,  $f_{nn}$  is the oscillator strength,  $E_1$  is the first energy state,  $E_2$  is the excited energy,  $E_g$  is the transition energy,  $E_f$  is the Fermi level, m<sup>\*</sup> is the effective mass of the well,  $L_w$  is the width of quantum well, c is the speed of light,  $n_r$  is the refractive index of the well.

The oscillator strength indicates the probability of an electron being excited from ground state to an excited state. It is found by [1]:

$$f = \frac{4\pi m \dot{\upsilon}}{\hbar} \langle Z \rangle^2 \qquad (13)$$

where  $\upsilon$  is the transition frequency, m<sup>\*</sup> is the effective mass of the well, and  $\langle Z \rangle$  is the dipole matrix element, which can be found from the wave function.

#### 3. Results and Discussion

By solving the Schroedinger equation, allowed energy levels and wave function can be determined. Figures 2a, 2b, 2c, and 3 illustrate the energy levels for embedded well structure with thick barrier, the superlattice, the embedded well structure with superlattice barrier, and the wave function of the embedded well, respectively. The results confirmed the bound-to-miniband transition and the location of the excited energy level within the miniband for the newly design embedded well structure.

The absorption coefficient for the structure is calculated to be 4.159E3 1/cm at 300 K and at the peak wavelength of 8.3  $\mu$ m. Figure 4 shows the absorption coefficient of the structure for different temperatures.

From the theoretical calculation, the InGaP/GaAs/AlGaAs embedded well structure shows promising results as a long wavelength infrared detector.



Figure 2 Position of the energy levels for a) well section b) superlattice barrier section c) the embedded structure



Figure 3 Wavefunction of the well section a) ground state b) first excited state



Figure 4 Absorption coefficient of the structure for different temperatures

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