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Red Shift in Optical Properties of Type-I $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ Nano-heterostructure under External Strain

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Red Shift in Optical Properties of Type-I $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ Nano-heterostructure under External Strain

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Abstract. The application of external pressure on a heterostructure produces changes in the lattice parameter and symmetry of the material. These in turn produce significant changes in the electronic bandstructure. Due to the application of external pressure energy gaps are altered. This paper reports the energy bandstructure, wavefunctions and optical gain in type-I $\text{n-Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16} / \text{p-Al}_{0.45}\text{Ga}_{0.55}\text{As}$ nano-heterostructures under uniaxial strain (-1 to +1 GPa) along [110] directions in the red visible region. Numerical calculations of the photonic energy and optical gain of TE and TM modes in GaAsP/AlGaAs laser diode structure have been carried out for various uniaxial strain at temperature 300 K. The band structure was calculated using 6×6 Luttinger-Kohn Hamiltonian to determine sub-band dispersion and corresponding wavefunctions. The Heterostructure is observed to operate in the energy range 1.62 to 1.78 eV (696 to 765 nm).

1. Introduction

Specification of the lasing wavelength and substrate material availability usually influence the active region material selection. In a quantum well heterostructure design for the active region, there are a number of parameters that need to be determined, including the number of quantum wells, the well thickness, the well band gap energy and the strain on the well (i.e., the well material composition), the barrier band gap energy and the strain on the barrier. Strain modifies the bandstructure and crystal symmetry of the semiconductor. The k.p method was used to specify conduction and valance band shift. In semiconductors, lattice mismatch, applied external stress leads to strain. For Optical gain, Hongping Zhao et. al demonstrated compensated InGaN-AlGaIn quantum well active regions for laser emitting at 420-500 nm. A calculation for reduction of threshold carrier density and current density for strain compensated InGaIn-AlGaIn quantum well active region has been presented. It was found that biaxial strain would enhance the optical gain and minimum peak gain is obtained under a small tensile strain [1]. E V Bogdanov et al. have studied p-AlGaAs/GaAsP/n-AlGaAs heterostructures and polarization mode switching has been reported under the application of compressive stress [2]. Mixing of wavefunction character between contiguous sub bands can be reduced by strained structure. [3]. In heterostructures optical transitions can be specified in terms of momentum matrix elements or dipole matrix elements [4].



The effect of Uniaxial strain and compression on optical properties of heterostructures have been investigated in several studies recently [5, 6, 7, 8, 9]. To know the bandstructure and the wavefunctions of bound and unbound states in both lattice matched and strained quantum well k.p method was used.

2. Structure & Theory

The active region consists of a single quantum well (5 nm) of $\text{GaAs}_{0.84}\text{P}_{0.16}$ material and the barrier layers consists of ternary alloys $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ and $\text{Al}_{0.7}\text{Ga}_{0.3}\text{As}$ (16 nm) The subband dispersion and corresponding wavefunctions were calculated using Luttinger-Kohn 6x6 model hamiltonion. Equilibrium and injected electrons/holes concentration were $1.6 \times 10^{12} / \text{cm}^2$ and $3.5 \times 10^{12} / \text{cm}^2$ respectively. The entire heterostructure was grown on the substrate of binary compound GaAs. For the calculations, both external and internal strains have been considered. Internal strain appears because of lattice mismatch of the layers. For the lattice mismatched strain, We consider

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_0 - a}{a}; \quad \epsilon_{zz} = \frac{2C_{12}}{C_{11}} \epsilon_{xx}$$

Where a and a_0 are the lattice constants of the layer and substrate. C_{12} and C_{11} are the stiffness constants. The energy band structure is shown in Fig. 1 with various energy bands. The type-I QW structure is based on GaAs substrate and has a of length 21 nm.

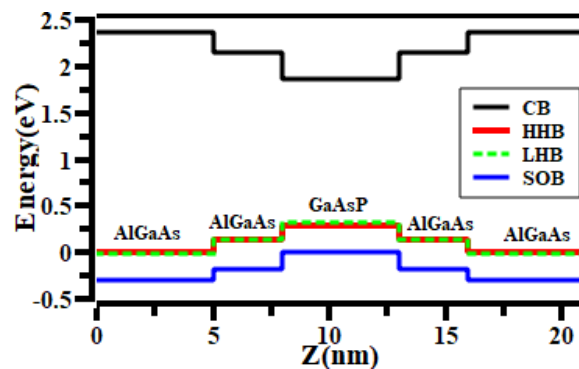


Figure. 1. Energy banddiagram of $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure.

The fundamental theory for the study of motion of holes and electron in perturbed fields is extensively presented [10,11,22,13,14]. The E-k dispersion curve of the structure calculation is the basis of succeeding computations. The block diagonalised system Hamiltonian is applied for the numerical computation of electronic energy bands and wavefunctions in the QW heterostructure.

For calculation of the optical gain coefficient of the nano-scale heterostructure, Fermi's golden rule is applied [15,16,17,18,19]. The valance and conduction band profiles and wavefunctions of electrons and holes for the type-I $\text{n-Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16} / \text{p-Al}_{0.45}\text{Ga}_{0.55}$ have been numerically calculated for various values of external pressure along [110] directions. Numerical calculations were performed with the help of HD studio software. Wavefunctions, Optical matrix element of electron photon interaction and momentum matrix element as well as optical gain in TM and TE mode for the type-I $\text{n-Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{p-Al}_{0.45}\text{Ga}_{0.55}$ were performed under external pressure up to 1 GPa along [110] directions at 300 K. Fig. 2, Fig.3 and Fig. 4 show the bandstructure and the wavefunctions of type I $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure [20,21,22].

In the following section the results from simulations are discussed.

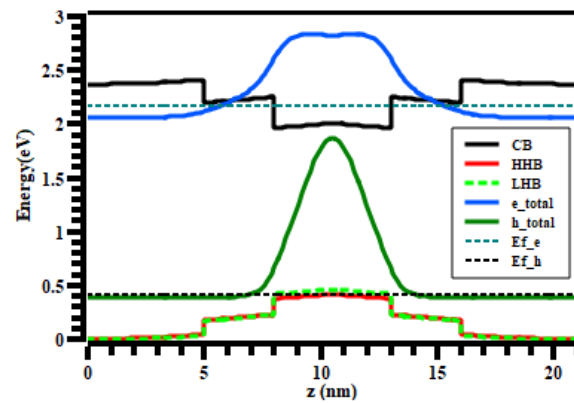


Figure 2. e-h (total) wavefunctions in $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure

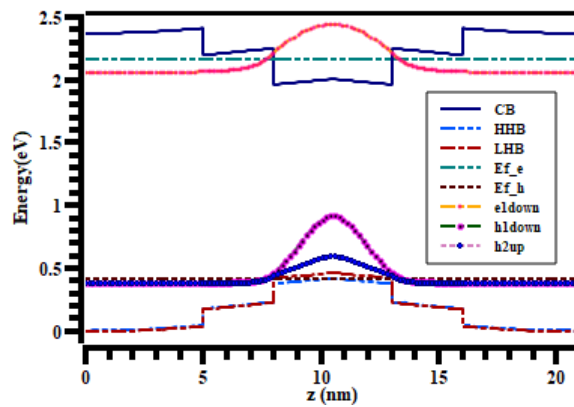


Figure 3. $e_1-h_1(\text{down})$ wavefunctions in $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure

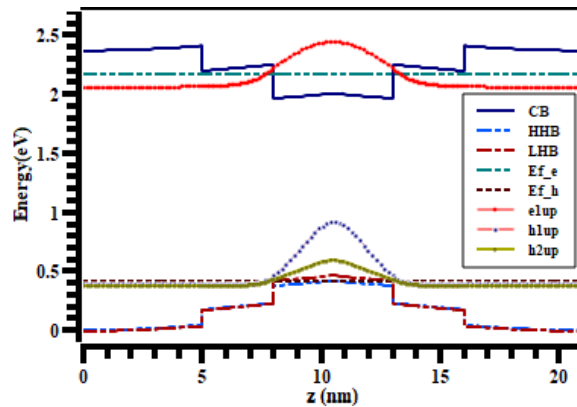


Figure 4. $e_1-h_1(\text{up})$ wavefunctions in $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure

3. Results & Discussion

This paper investigates the effect of external pressure on optical gain associated with the optical matrix element for a 5nm n- $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{p-Al}_{0.45}\text{Ga}_{0.55}$ quantum well along with [110] direction at temperature 300 K. To investigate the optical gain in n- $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{p-Al}_{0.45}\text{Ga}_{0.55}$ type-I nanoscale heterostructure, initially the Schrodinger equation was solved for finding the wavefunctions related to conduction band whereas six band hamiltonian was solved to find out the wavefunctions related to valance subbands. After wavefunction determination, energy band dispersion for conduction band electrons and valance band holes were calculated. The 6×6 Luttinger-Kohn model and self-consistent calculations is used for computation of wavefunctions of the structure. For this e_1-h_1 and e_1-h_2 transitions are selected for computation in this present case.

The application of external pressure on a heterostructure produces changes in the lattice parameter and symmetry of the material. These in turn produce significant changes in the electronic band structure. Due to the application of the external pressure energy gaps was altered. Effective masses are affected by change in the interband matrix elements and variations in the energy gaps.

The optical gain in z polarization as well width variations is shown in Fig. 5. Optical gain is computed on various strains (-0.5, -1, 0, 1, 0.5 GPa) at 300K. The optical gain of the heterostructure under z polarization is 4177/cm under no pressure condition. A right shift is also observed in the optical gain spectrum for increasing compression. A left shift along with a drop is observed in the optical gain spectrum for increasing tensile strains.

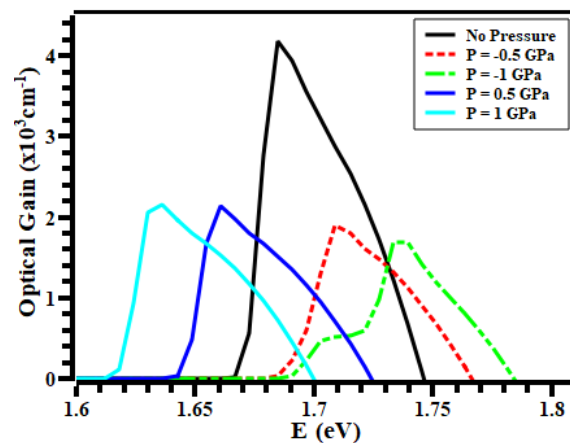


Figure 5. Optical Gain spectra of $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure as strain variations along [110] direction at $T=300\text{ K}$

4. Conclusion

This paper reports the analysis of optical matrix element and optical gain in $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}$ heterostructure along the [110] directions. Initially, the wavefunctions associated with the conduction and valance band, energy band dispersion for conduction band electrons and valance band holes, matrix elements and finally optical gain have been computed under different strain conditions. Equilibrium and injected electron/hole charge carrier concentration were 1.6 & 3.5 ($\times 10^{12}\text{ cm}^{-2}$). The band structure was calculated using 6×6 Luttinger-Kohn Hamiltonian to determine sub-band dispersion and corresponding wavefunctions. This heterostructure is observed to operate in the energy range 1.62 to 1.78 eV (696 to 765 nm). Based on the outcomes it is realised that the optical gain of the $\text{InGaAs}/\text{GaAsP}$ heterostructure can be suitably red shift tuned as per the requirements.

Overall comparison between Energy (eV), gain, wavelength at different strain along the [110] directions are shown in table 1. It shows the red shift tuning of the $\text{InGaAs}/\text{GaAsP}$ heterostructure on different strain.

Table 1. Comparison of Energy (eV), gain, wavelength at different strain along the [110] directions

Strain [110]	E (eV)	Gain (max)	λ (nm)
-1	1.739	1688	712.96
-0.5	1.7	1903	729.3
0	1.684	4177	736.24
0.5	1.66	2141	746.89
1	1.636	2157	757.84

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