Red Shift in Optical Properties of Type-I
Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$/Al$_{0.45}$Ga$_{0.55}$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 n-Al$_{0.45}$
Ga$_{0.55}$ As/GaAs$_{0.84}$P$_{0.16}$ / p-Al$_{0.45}$ Ga$_{0.55}$ 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-AlGaN 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 InGaN-AlGaN 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 GaAs$_{0.84}$P$_{0.16}$ material and the barrier layers consists of ternary alloys Al$_{0.45}$Ga$_{0.55}$As and Al$_{0.7}$Ga$_{0.3}$As (16 nm) The subband dispersion and corresponding wavefunctions were calculated using Luttinger-Kohn 6x6 model hamiltonian. Equilibrium and injected electrons/holes concentration were $1.6 \times 10^{12}$/cm$^2$ and $3.5 \times 10^{12}$/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

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

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.

![Energy band diagram](image)

**Figure. 1.** Energy banddiagram of Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$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 n-Al$_{0.45}$ Ga$_{0.55}$ As/GaAs$_{0.84}$P$_{0.16}$/p-Al$_{0.45}$ 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 n-Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$/p-Al$_{0.45}$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 Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$ heterostructure [20,21,22].

In the following section the results from simulations are discussed.
Figure 2. e-h (total) wavefunctions in Al$_{0.45}$Ga$_{0.55}$As/ GaAs$_{0.84}$P$_{0.16}$ heterostructure

Figure 3. e$_1$-h$_1$(down) wavefunctions in Al$_{0.45}$Ga$_{0.55}$As/ GaAs$_{0.84}$P$_{0.16}$ heterostructure

Figure 4. e$_1$-h$_1$ (up) wavefunctions in Al$_{0.45}$Ga$_{0.55}$As/ GaAs$_{0.84}$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-Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$/p-Al$_{0.45}$Ga$_{0.55}$ quantum well along with [110] direction at temperature 300 K. To investigate the optical gain in n-Al$_{0.45}$Ga$_{0.55}$As/GaAs$_{0.84}$P$_{0.16}$/p-Al$_{0.45}$Ga$_{0.55}$ type-I nanoscale heterostructure, initially the Schrodinger equation was solved for finding the wavefunctions related to conduction band where as 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 6x6 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 Al0.45Ga0.55As/ GaAs0.84P0.16 heterostructure as strain variations along [110] direction at T=300 K](image)

4. Conclusion
This paper reports the analysis of optical matrix element and optical gain in Al0.45Ga0.55As/GaAs0.84P0.16 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. Equilbrium and injected eletron/hole charge carrier concentration were 1.6 & 3.5 ($ \times 10^{12} $ cm$^{-2}$ ). The band structure was calculated using 6x6 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 InGaAs/GaAsP heterostructure can be suitably red shift tuned as per the requirements.

Overall comparision 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 InGaAs/GaAsP heterostructure on different strain.

| Strain [110] | E (eV) | Gain (max) | $\lambda$ (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         |
5. References

[1] Hongping Zhao, Ronald A. Arif “Optical gain analysis of strain-compensated InGaN-AlGaN quantum well active regions for laser emitting at 420-500nm. Opt Quant Electron (2008) 40:301-306

[2] E V Bogdanov, K I Kolokolov, N V Melnikova, N Ya Minina and G V Tikhomirova, “Polarization mode switching in p-AlGaAs/GaAsP/n-AlGaAs diodes in presence of compressive stress”, IOP Conf. Series: Journal of Physics: Conf. Series 950 (2017) 042047

[3] Wood, A.C.G., “Strain effects in Semiconductor quantum wells”, PhD thesis, Durham University, Sept 1990.

[4] B.G.U, N.H Kwong, “Relation between Interband Dipole and momentum matrix elements in Semiconductor” physical review. B, Condensed matter March 2013

[5] H. K. Nirmal, S. G. Anjum, Pyare Lal, Amit Rath, S. Dalela, M. J. Siddiqui, P. A. Alvi, “Field effective band alignment and optical gain in type-I Al0.4Ga0.55As/GaAs0.84P0.16 nano-heterostructures”, International Journal of light and electron optics: Optik 127,7274-7282 (2016).

[6] Md. Riyaj, A.K. Singh, Amit Rath, Sandhya Kattayat, Shalendra Kumar, S Dalela, P.A. Alvi, “High Pressure affects on Optical Characteristics of AlGaAs/GaAsP/AlGaAs nano-heterostructure”, Optik, Volume 181, March 2019, Pages 389-397, Elsevier, Dec. 2018.

[7] A. K. Singh, Amit Rath, Md. Riyaj, P.A. Alvi, “Optical gain tuning within IR region in type-II In0.4Gao.55As/P0.2/GaAs0.5Sb0.5 nano-scale heterostructure under external uniaxial strain”, Superlattices and Microstructures 98 (2016) , Elsevier, June 2017.

[8] A. K. Singh, Md. Riyaj, S.G. Anjum, Nisha Yadav, Amit Rath, M.J. Siddiqui, P.A. Alvi, “Anisotropy and optical gain improvement in type-II In0.4Ga0.55As/GaAs0.4Sb0.6 nano-scale heterostructure under external uniaxial strain”, Superlattices and Microstructures 98 (2016), Elsevier, June 2016, Volume 98, October 2016, Pages 406–415.

[9] Vibha Kumari, Ashish, Swati Jha, Amit Rath, H. K. Nirmal, P. A. Alvi, “Optical Gain of InGaAlAs Quantum well with Different Barriers, Claddings and Substrates”, Journal of Optoelectronics Engineering, Science and Education Publishing, 2014, Vol. 2, No. 2, pp. 42-45

[10] J.M. Luttinger, W. Kohn, “Motion of electrons and holes in perturbed periodic fields”, Physical Review 97 (4) (1955) 869.

[11] Wallace C. H. Choy, Tailoring Light and Heavy Holes of GaAsPAlGaAs Quantum Wells by Using Interdiffusion for Polarization - Independent Amplifier Applications, IEEE Journal of Quantum Electronics, Vol. 36, No. 2, February 2000.

[12] J.M. Luttinger, Quantum theory of cyclotron resonance in semiconductors: general theory, Physical Review 102 (4) (1956) 1030.

[13] Paul Harrison, Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures, John Wiley & Sons, 2005.

[14] Shun Lien Chuang, Physics of Optoelectronic Devices, John Wiley & Sons, 1995.

[15] Chih-Sheng Chang, Shun Lien Chuang, “Modeling of strained quantum well lasers with spin-orbit coupling”, IEEE Journal of Selected Topics in Quantum Electronics I (2) (1995) 218-229.

[16] Amit Rathi , Amit Kumar Singh, “Optical Response Computations in Type-II Doped AlSb/InAs Nano-Heterostructure under External uniaxial strain in SWIR Range”, IEEE 3rd International Conference on Engineering, Technologies and Social Sciences, (2017), ISBN No.-978-1-5386-1611-6.

[17] Jirgen Sebastian, Gert Beister, Frank Bugge, E. Buhrandt, Goetz Erbert, H. G. Hansel, R. Hulswede et al., High-power 810-nm GaAsP-AlGaAs diode lasers with narrow beam divergence, IEEE Journal of Selected Topics in Quantum Electronics 7, no. 2 (2001): 334-339.

[18] Md. Riyaj, A. K. Singh, Sandhya K., Amit Rathi, P. A. Alvi, Optical properties of Type-I GaAsP-AlGaAs nano-heterostructure under external uniaxial strain, In AIP Conference
Proceedings, vol. 1832, no. I, p. 120022. AIP Publishing, 2017.

[19] Hidenao Tanaka, Jun-ichi Shimada, and Yoshio Suzuki, Highly efficient TE/TM mode switching of GaAsP/AlGaAs strained quantum-well laser diodes, Applied physics letters 64, no. 2 (1994): 158-160.

[20] E.V. Bogdanov, H. Kissel, K.I. Kolokolov, N. Ya Minina, TM/TE polarization tuning and switching in tensile strained pAlGaAs/ GaAsP/n-AlGaAs heterostructures by uniaxial compression, Semiconductor Science and Technology 31 (3) (2016) 035008.

[21] E.V. Bogdanov, N. Ya Minina, J.W. Tomm, H. Kissel, Effect of uniaxial stress on electroluminescence, valence band modification, optical gain, and polarization modes in tensile strained p-AlGaAs/GaAsP/n-AlGaAs laser diode structures: numerical calculations and experimental results, Journal of Applied Physics 112 (9) (2012) 093113.

[22] E.V. Bogdanov, N. Ya Minina, S.S. Shirokov, A.E. Yunovich, H. Kissel, Electroluminescence in laser diode nanostructures p-AlxGa1-xAs/ GaAs1-yPy/n-AlxGal_xAs under uniaxial compression, in: Physics, Chemistry and Application of Nanostructures: Reviews and Short Notes, 2009, pp. 609-612.

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