

## **Study of Nano-Hetrostructure of Type-Ii Compound Semiconductors: Their Electronic and Hole Wave Function Action in Mid Infrared Region**

**S F Haider<sup>2</sup>, R Sharma<sup>1#</sup>, P A Alvi<sup>2</sup>, S K Gupta<sup>2</sup>, S Sharma<sup>3</sup>,**

<sup>1</sup>.*Department of Physics, National Defence Academy Khakwasla Pune Maharashtra 411023.*

<sup>2</sup>.*Department of Physics, Banasthali Vidyapith, Banasthali Rajasthan 304022*

<sup>3</sup>.*Omega College of Professional Studies, Station Road Freeganj Ujjain 456010*  
(# Corresponding Author). E-Mail: [rakesh\\_sharma\\_ujn@yahoo.co.in](mailto:rakesh_sharma_ujn@yahoo.co.in)

### **Abstract**

A nano-hetrostructure of W shaped type-II compound semiconductor which have combination of layers made by AlSb, InAs and GaAsSb is studied for utilization in Lasing action of Mid Infrared Region (MIR). For this heterostructure, a multiband band k.p Hamiltonian has been simplified to compute the required carrier's wave functions, their subband structures and matrix dipole elements accountable for the probabilistic transitions which results into the high optical gain. For 2-D charge carrier density of  $1.5 \times 10^{12} \text{ cm}^{-2}$ , the computed results confirm that only the light hole (LH) subbands take part in optical transition in order to produce the high optical gain of the order of  $\sim 8850 / \text{cm}$  which corresponds to  $\sim 5.2 \mu\text{m}$ . Keeping in view its high optical gain at  $\sim 5.2 \mu\text{m}$ , the proposed type-II AlSb/InAs/GaAsSb heterostructure can be of use in the environmental monitoring, particularly important for sensing the CO<sub>2</sub>, CO and NO lethal gases available in the contaminated environment.

### **1. Introduction:**

The researchers of the field of optoelectronics are paying attention on quantum well (QW) heterostructures as these structures have potential utilization in the field of infrared detectors, MIR spectroscopy, gas leakage sensing, optical data transferring, MIR emitters and monitoring of pollution

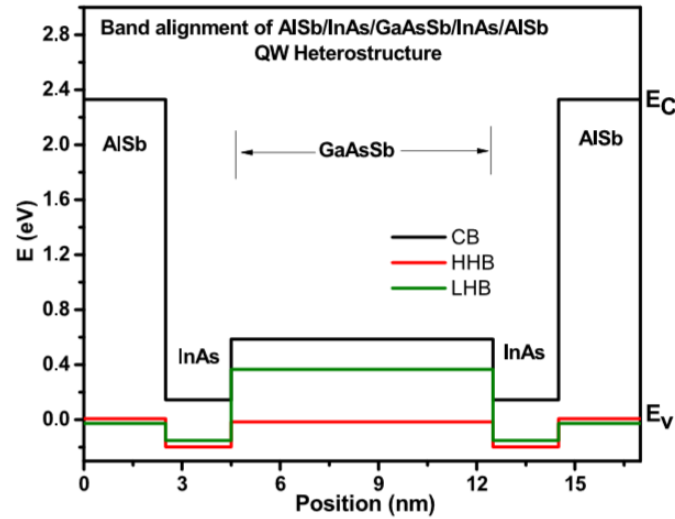
[Ohno et al., 1992; Duggan and Ralph, 1987; Nirmal et al., 2015; Yadav et al., 2017; Alvi, 2017; Singh et al., 2017; Dolia et al., 2017]. These QW have a very remarkable role in tunable semiconductor lasers which have yield of 3-5  $\mu\text{m}$ . These lasers are used in surgery, medical diagnosis and pollution monitoring.[ Bandyopadhyay et al., 2012;

Tian et al., 2012; Bewley et al., 2012]. The tunable semiconductor lasers, which emit MIR radiations in continuous-wave mode at room temperature, play a key role in gas sensing analysis by making use of absorption spectroscopy. This is because, the several fundamental absorption lines of industrial and natural gases, such as carbon monoxide (CO), hydrocarbons, nitrous oxide (N<sub>2</sub>O), carbon dioxide (CO<sub>2</sub>), ammonia (NH<sub>3</sub>) and formaldehyde are available in this spectral range. In most of the studies of optoelectronic devices working as infrared detectors are investigated for use in intersubband transition [Goossen et al., 1988; Ryczko et al., 2015; Kang et al., 1989]. But, there is some major trouble in making use of intersubband transitions in an actual device. The basic problem with intersubband transitions is related to efficiently injection of carriers into and removing them out of the desired subbands for light emission with high efficiency. The QWs based heterostructures utilizing the interband transitions can be suggested, which can emit or detect the light beam with higher efficiency. They are best utilize in production of cascade laser by Ryczko et al and Motyka et al in their work [Ryczko et al., 2015; Motyka et al., 2016]. This laser have potential application in sensing of toxic gases and analysis of human breathe. [Yang, 1995; Vurgaftman et al., 2015]. The other attractive features of these laser sources are low threshold currents which result in small power consumption and wide-ranging spectral tunability with in the mid-infrared wavelength region [Vurgaftman et al., 2011; Jiang et al., 2014]. In this article, a unique and proper combination of AlSb, InAs and GaAsSb layers is described to optimize the W-shaped type-II QW heterostructure considering its growth on GaSb substrate with the utilization of interband transitions, which can be beneficial for family of optoelectronic devices, particularly, interband cascade laser sources emitting the MIR radiations with higher efficiency. For example, the InAs/AlSb heterointerface based heterostructure containing multilayers have been utilized in formation of quantum cascade lasers (QCLs) due to the large conduction band discontinuity of 2.1 eV, beneficial for fabrication of short wavelength QCLs, and a moderate lattice mismatch between these compounds [Nicolai et al., 2014]. Even, a lot of study has been carried out on the AlSb/InAs/GaAsSb Type-II quantum well heterostructure; there are still some fundamental characteristics, which are required for such new heterostructures that may be beneficial for tunable interband cascade laser sources for MIR emission.

## **2. Heterostructure design:**

The proposed heterostructure has a proper combination of AlSb, InAs and GaAsSb layers in such a way that it forms a type-II (broken type) W-shaped heterostructure comprising of two QWs of InAs layer (2 nm) separated by a GaAsSb layer (8 nm), see Fig. 1. The composition of the GaAsSb layer is specified as GaAs<sub>0.65</sub>Sb<sub>0.35</sub>. The AlSb layer works as a barrier layer. Moreover, the uniqueness of this W-shaped type-II QW heterostructure is that the conduction band (CB) of InAs layer is lower than the valence subband (light hole) in valence band (VB) of GaAsSb layer, due to which the interface between InAs and GaAsSb layers creates type-II hetero-junction. Due to this hetero-interface uniqueness, such type-II heterostructures can also be useful in designing of interband tunnel diodes. Also, the energy bandgap of AlSb layer covers

the bandgap of GaAsSb layer and some region of the bandgap of the InAs layer. The growth of this QW heterostructure has been considered on the GaSb substrate, as already reported in literature its potential applications and performance in IR region [Liu et al., 2018].



**Fig 1** Band alignment with schematic layers arrangement of AlSb/InAs/GaAsSb type-II QW heterostructure

In order to analyse the AlSb/InAs/GaAsSb type-II QW heterostructure in context of behaviour of carriers (electrons and holes) wavefunctions, corresponding energy levels of carriers, the dispersion (E-K) curves, dipole matrix elements and optical gain, a traditional quantum mechanics has become very helpful. Since, the proper information of carrier's wavefunction associated with the conduction and valence subbands is needed for the dipole matrix elements of the required and allowed transitions and optical gain characteristics; therefore six bands k.p theory in quantum mechanics including the strain effects has been adopted for collecting such informative results. To obtain the standard parameter  $6 \times 6$  Luttinger-Kohn Hamiltonian is solved [S.Feroz Haider et al 2021].

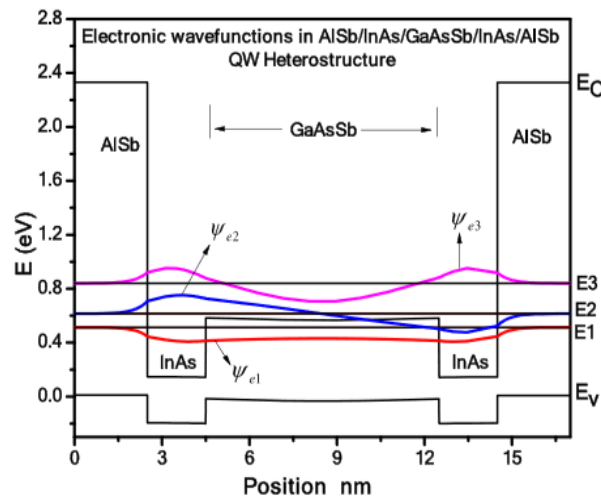
**Table-1**

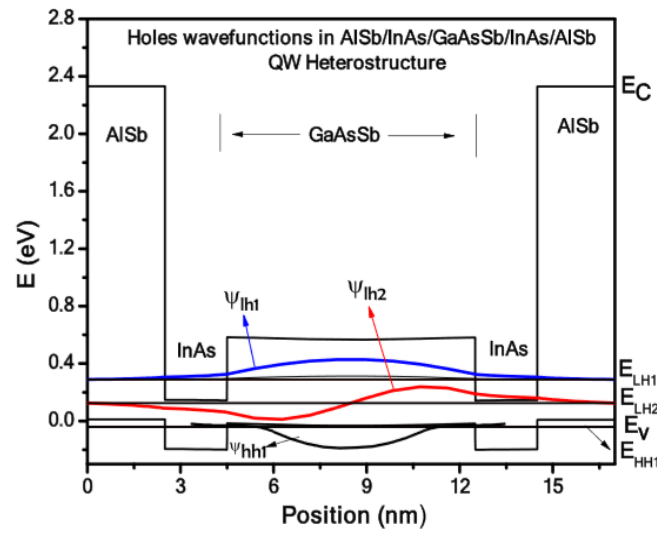
Parameters (Luttinger parameters) of material used in heterostructure.

Parameters	GaSb	AlSb	GaAs	InAs
$\gamma_1$	13.4	5.18	6.98	20.0
$\gamma_2$	4.7	1.19	2.06	8.50
$\gamma_3$	6.00	1.97	2.93	9.20
$m_{\frac{1}{2}}^*/m_0$	0.039	0.14	0.067	0.024
$m_{HH}^*/m_0$	0.37	0.28	0.55	0.36
$m_{LH}^*/m_0$	0.043	0.05	0.083	0.026
$m_{SO}^*/m_0$	0.12	0.13	0.165	0.014

**3. The analysis of characteristics of Type II QW Heterostructure:** In this section a detailed analysis of Type II QW heterostructure is presented based on simulation results.

**3.1 The Wavefunction:** The fig 2 and fig 3 present calculated wave function of AlSb/InAs/GaAsSb Type II QW heterostructure. . In order to make theoretically testing and understanding the mechanism of producing the high optical gain, we analysed the AlSb/InAs/GaAsSb type-II W-shaped QW heterostructure successfully. This heterostructure has a proper combination of coupled double QWs of InAs layer separated by GaAsSb ternary layer, where the ternary confinement layer is strained tensely for holes.

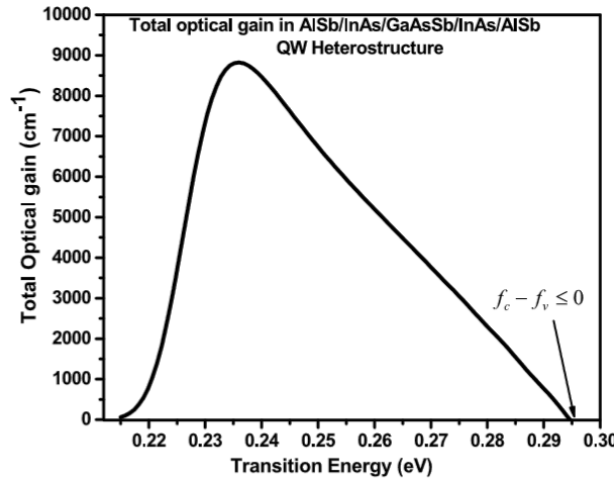
**Fig 2** Illustration of Calculated electronic wavefunctions in Type II QW



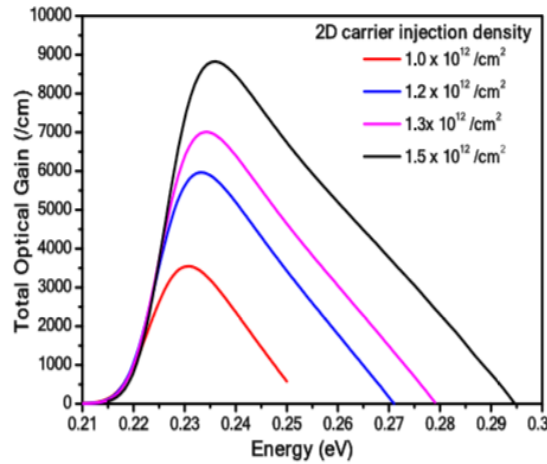
**Fig 3-**Illustration of calculated holes wavefunctions in Type II QW

However, to find the optimized optical gain characteristics of the heterostructure, the prior information of carrier's wavefunctions, and their optical transitions obeying the restricted selection rules are very essential. These hole's wavefunctions represent that the holes are highly localized and hence confined only in the spacer region (GaAsSb layers).

**3.2 Optical Gain:** In fig 4 the estimated optical gain characteristic of the type-II AlSb/InAs/GaAsSb QW heterostructure has been plotted as function of transition energy. Refer to the fig 4 the magnitude of achieved peak optical gain for the type-II AlSb/InAs/GaAsSb QW heterostructure is of the order of  $\sim 8850$  /cm which corresponds to 0.235 eV photonic energy resulting from transitions between electronic and hole subbands; the condition  $(f_c - f_v) \leq 0$  has also been mentioned at appearance of zero optical gain. Because of a well-known fact that the appearance of optical gain is only conceivable when the required condition  $(f_c - f_v) > 0$  is satisfied, otherwise the gain will not exist.



**Fig 4** The total optical gain of Type II QW heterostructure



**Fig 5** Total optical gain in 2D carrier injection Density

2D injected carrier's charge density dependent optical gain spectra have been studied and shown in Fig. 5. The plot of gain spectra shown in Fig. 5 confirm that the optical gain can be enhanced with increasing the carrier's charge injection. Further, the injected charge density can also help the gain spectra to shift in the longer wavelength region. Further, the wavelength ( $\sim 5.2 \mu\text{m}$ ) belongs to MIR region and has many important applications.

**4. Conclusion:** The type-II (with broken bandgap) W-shaped AlSb/InAs/GaAsSb heterostructure has been projected and deliberate by utilizing a simple six band k.p Hamiltonian in order to compute the required carrier's wavefunctions, their subband structures (i.e. dispersion relations) and matrix dipole elements responsible for the probabilistic transitions which consequences into the high optical gain. The computed outcome have confirmed that only the light hole subbands take part in optical

transition to produce the high optical gain of the order of  $\sim 8850/\text{cm}$  which corresponds to  $\sim 5.2 \mu\text{m}$ . Keeping in view the accessibility of high optical gain at  $\sim 5.2 \mu\text{m}$ , the proposed type-II AlSb/InAs/GaAsSb heterostructure can be beneficial in the environmental monitoring. The above mentioned heterostructure can be utilize in traditional application in Industrial, Medical, MIR spectroscopy and telecommunications application as they require 5200 nm wavelength.

### **Acknowledgement:**

The authors of this paper acknowledge DST for providing computational support through CURE at Banasthali Vidyapith, authors are very grateful to organizers of Christian Eminent College and Research Foundation of India to provide us platform to present our research at International Conference “Physics @ World: Contemporary and Innovative Applications-2021”.

### **Reference:**

#### **(In order of appearance)**

- [1] Ohno, H., Esaki, L., Mendez, E.E., 1992. Optoelectronic devices based on type II polytype tunnel heterostructures. *Appl. Phys. Lett.* 60, 3153–3155. <https://doi.org/10.1063/1.106726>.
- [2] Duggan, G., Ralph, H.I., 1987. Exciton binding energy in type-II GaAs-(Al, Ga)As quantum-well heterostructures. *Phys. Rev. B.* 35, 4152–4154. <https://doi.org/10.1103/PhysRevB.35.4152>.
- [3] Nirmal, H.K., Yadav, N., Lal, P., Alvi, P.A., 2015. Optical gain in type-II InGaAs/GaAsSb quantum well nano-heterostructure. *AIP Conf. Proc.* 1675, 3–7. <https://doi.org/10.1063/1.4929254>.
- [4] Yadav, N., Bhardwaj, G., Anjum, S.G., Dalela, S., Siddiqui, M.J., Alvi, P.A., 2017. Investigation of high optical gain in complex type-II InGaAs/InAs/GaAsSb nano- scale heterostructure for MIR applications. *Appl. Opt.* 56, 4243. <https://doi.org/10.1364/AO.56.004243>.
- [5] Alvi, P.A., 2017. Transformation of type-II InAs/AlSb nanoscale heterostructure into type-I structure and improving interband optical gain. *Phys. Status Solidi Basic Res.* 254, 1600572. <https://doi.org/10.1002/pssb:201600572>.
- [6] Singh, A.K., Rath, A., Riyaj, M., Bhardwaj, G., Alvi, P.A., 2017. Optical gain tuning within IR region in type-II In<sub>0.5</sub>Ga<sub>0.5</sub>As<sub>0.8</sub>P<sub>0.2</sub>/GaAs<sub>0.5</sub>Sb<sub>0.5</sub> nano-scale heterostructure under external uniaxial strain. *Superlattices Microstruct.* 111, 591–602. <https://doi.org/10.1016/j.spmi.2017.07.014>.
- [7] Dolia, R., Bhardwaj, G., Singh, A.K., Kumar, S., Alvi, P.A., 2017. Optimization of Type-II ‘W’ shaped InGaAsP/GaAsSb nanoscale-heterostructure under electric field and temperature. *Superlattices Microstruct.* 112, 507–516. <https://doi.org/10.1016/j.spmi.2017.10.007>.
- [8] Bandyopadhyay, N., Bai, Y., Tsao, S., Nida, S., Slivken, S., Razeghi, M.,

2012. Room temperature continuous wave operation of  $\lambda \sim 3\text{--}3.2\mu\text{m}$  quantum cascade lasers. *Appl. Phys. Lett.* <https://doi.org/10.1063/1.4769038>.
- [9] Tian, Z., Li, L., Ye, H., Yang, R.Q., Mishima, T.D., Santos, M.B., Johnson, M.B., 2012. InAs-based interband cascade lasers with emission wavelength at  $10.4\mu\text{m}$ . *Electron. Lett.* <https://doi.org/10.1049/el.2011.3555>.
- [10] Bewley, W.W., Canedy, C.L., Kim, C.S., Kim, M., Merritt, C.D., Abell, J., Vurgaftman, I., Meyer, J.R., 2012. High-power room-temperature continuous-wave mid-infrared interband cascade lasers. *Opt. Express.* 20, 20894. <https://doi.org/10.1364/OE.20.020894>.
- [11] Bewley, W.W., Canedy, C.L., Kim, C.S., Kim, M., Merritt, C.D., Abell, J., Vurgaftman, I., Meyer, J.R., 2012. Continuous-wave interband cascade lasers operating above room temperature at  $\lambda = 47\text{--}56\mu\text{m}$ . *Opt. Express.* 20, 3235–3240. <https://doi.org/10.1364/oe.20.003235>.
- [12] Goossen, K.W., Lyon, S.A., Alavi, K., 1988. Photovoltaic quantum well infrared detector. *Appl. Phys. Lett.* 52, 1701–1703. <https://doi.org/10.1063/1.99022>.
- [13] Ryczko, K., Sęk, G., Misiewicz, J., 2015. Novel design of type-II quantum wells for mid- infrared emission with tensile-strained GaAsSb layer for confinement of holes. *Appl. Phys. Express.* 8, 121201 <https://doi.org/10.7567/APEX.8.121201>.
- [14] Kang, P., Wang, L., Yuh, 1989. Theory superlattices. *IEEE J. Quantum Electron.* 25, 12–19.
- [15] Motyka, M., Dyksik, M., Ryczko, K., Weih, R., Dallner, M., Höfiling, S., Kamp, M., Sęk, G., Misiewicz, J., 2016. Type-II quantum wells with tensile-strained GaAsSb layers for interband cascade lasers with tailored valence band mixing. *Appl. Phys. Lett.* 108, 101905 <https://doi.org/10.1063/1.4943193>.
- [16] Yang, R.Q., 1995. Infrared laser based on intersubband transitions in quantum wells. *Superlattices Microstruct.* 17, 77–83. <https://doi.org/10.1006/spmi.1995.1017>.
- [17] Vurgaftman, I., Bewley, W.W., Canedy, C.L., Kim, C.S., Kim, M., Merritt, C.D., Abell, J., Lindle, J.R., Meyer, J.R., 2011. Rebalancing of internally generated carriers for mid- infrared interband cascade lasers with very low power consumption. *Nat. Commun.* 2, 585. <https://doi.org/10.1038/ncomms1595>.
- [18] Vurgaftman, I., Weih, R., Kamp, M., Meyer, J.R., Canedy, C.L., Kim, C.S., Kim, M., Bewley, W.W., Merritt, C.D., Abell, J., Höfiling, S., 2015. Interband cascade lasers, *J. Phys. D: Appl. Phys.* 48, 123001 <https://doi.org/10.1088/0022-3727/48/12/123001>.
- [19] Jiang, Y., Li, L., Tian, Z., Ye, H., Zhao, L., Yang, R.Q., Mishima, T.D., Santos, M.B., Johnson, M.B., Mansour, K., 2014. Electrically widely tunable interband cascade lasers. *J. Appl. Phys.* 115, 113101 <https://doi.org/10.1063/1.4865941>.
- [20] Jiang, Y., Li, L., Yang, R.Q., Gupta, J.A., Aers, G.C., Dupont, E., Baribeau, J.M., Wu, X., Johnson, M.B., 2015. Type-I interband cascade lasers near  $3.2\mu\text{m}$ . *Appl. Phys. Lett.* 106, 041117 <https://doi.org/10.1063/1.4907326>.



- [21] Nicolai, J., Gatel, C., Warot-Fonrose, B., Teissier, R., Baranov, A.N., Magen, C., Ponchet, A., 2014. Elastic strains at interfaces in InAs/AlSb multilayer structures for quantum cascade lasers. *Appl. Phys. Lett.* 104, 031907. <https://doi.org/10.1063/1.4863035>.
- [22] Liu, A.W.K., Lubyshev, D., Fastenau, J.M., Nelson, S., Kattner, M., Frey, P., 2018. Molecular beam epitaxial growth and characterization of large-format GaSb-based IR photodetector structures [Invited]. *Opt. Mater. Express.* 8, 1282. <https://doi.org/10.1364/OME.8.001282>.
- [23] Syed Firoz Haider, Upendra Kumar, Sandhya Kattayat, Smitha Josey, M. Ayaz Ahmad, Saral K. Gupta, Rakesh Sharma, Mohammed Ezzeldieng, P.A. Alvi, *Results in Optics* 5 (2021) 100138. [doi.org / 10.1016 / j.rio.2021.100138](https://doi.org/10.1016/j.rio.2021.100138).

