International Journal of Advanced Engineering Research and Science (IJAERS)
Peer-Reviewed Journal
ISSN: 2349-6495(P) | 2456-1908(O)
Vol-11, Issue-4; Apr, 2024
Journal Home Page Available: https://ijaers.com/
Article DOI: https://dx.doi.org/10.22161/ijaers.114.14

Design and Simulation of InGaAs/GaAsSb single quantum well structure for optical fiber application: Electronic Band Structure, Carrier Transport, and Optical Gain Analysis

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Received: 05 Feb 2024,

Receive in revised form: 20 Mar 2024,

Accepted: 01 Apr 2024,

Available online: 10 Apr 2024

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***Keywords*— Quantum well structure, Optical gain, WDM/DWDM**

***Abstract*— This paper explores the electronics and optical gain characteristics of an InGaAs/GaAsSb single quantum well structure designed on a GaAs substrate at room temperature (300 K). The findings indicate that this structure can emit radiation at 1550 nm with a significantly higher gain of approximately 6300/cm, rendering it suitable for optical fiber communication and optics applications such as WDM/DWDM for long-haul fiber transmission. This work contributes to advancing the field of optoelectronics by providing a promising solution for efficient NIR wavelength emission with substantial optical gain.*

I. INTRODUCTION

Optoelectronic devices utilizing compound semiconductors have revolutionized modern technology, enabling the development of high-performance systems for various applications, including telecommunications, data transmission, and sensing [1-3]. At the heart of these devices lies the intricate design of heterostructures, where different semiconductor materials with tailored properties are intricately combined to achieve specific functionalities [4]. The synergistic integration of various materials within heterostructures offers unparalleled opportunities to manipulate electronic and optical properties, paving the way for the creation of novel optoelectronic devices with enhanced performance characteristics. Compound semiconductors, such as InGaAs, GaAsSb, and related alloys, are particularly favored for optoelectronic applications due to their unique optical and electrical properties, including direct bandgaps, high electron mobilities, and compatibility with lattice-matched substrates [5-9]. These materials serve as the building blocks for the construction of heterostructures, where precise control over layer thickness, composition, and doping profiles is crucial to tailor the device's optical and electronic properties. The design of heterostructures for optoelectronic devices involves intricate considerations, including band alignment engineering, carrier confinement, and optical gain optimization [10]. By judiciously selecting materials and layer configurations, researchers can tailor the band structure to achieve desired electronic and optical characteristics, such as efficient carrier transport, enhanced light-matter interaction, and high optical gain. Advanced simulation tools, such as density functional theory (DFT), empirical pseudopotential method (EPM), and finite element methods (FEM), play a crucial role in predicting and optimizing the performance of heterostructures prior to fabrication [11]. In this context, this paper presents a comprehensive overview of the design and simulation of heterostructures for optoelectronic devices using compound

semiconductors. We delve into the fundamental principles governing the electronic band structure, carrier transport mechanisms, and optical gain characteristics of heterostructures, highlighting the latest advancements and challenges in this rapidly evolving field. Through a detailed examination of the design considerations and simulation methodologies, we aim to provide valuable insights into the development of next-generation optoelectronic devices with enhanced performance and functionality.

II. DESIGN SPECIFICATIONS AND STRUCTURAL INFORMATION

In this study, we focus on designing and modeling a nanoscale structure composed of layers of materials InGaAs/GaAsSb to analyze the computation of energy wave functions and optical gain. Understanding the lasing characteristics of the proposed heterostructure necessitates a thorough understanding of bulk materials, which serve as the foundation for studying nanoscale structures. Figures 1 and 2 depict the band structure diagrams of the ternary materials InGaAs and GaAsSb, respectively, at room temperature (300 K). The valence band of these materials comprises three bands: the heavy-hole band (HHB), thelight-hole band (LHB), and the split-off sub-band (SOB), distinguished based on their effective mass.

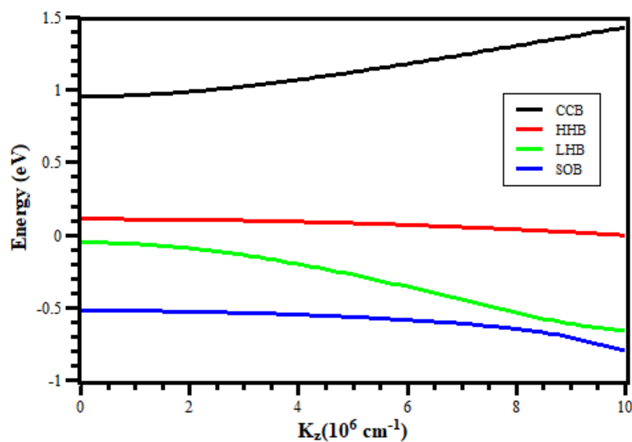

Fig.1. Band constructions of ternary compound InGaAs / GaAs

The heavy hole sub-band exhibits a higher effective mass compared to the light hole sub-band, while the light hole bands demonstrate a steeper energy slope than the heavy hole bands. The split-off band, positioned considerably below the conduction band, holds minimal significance due to its negligible energy. A prevalent challenge in semiconductor lasers lies in the elevated effective mass of the valence band. This issue is particularly common in group III-V semiconductors, stemming from a notable imbalance in the effective masses of charge carriers between the valence and conduction bands.

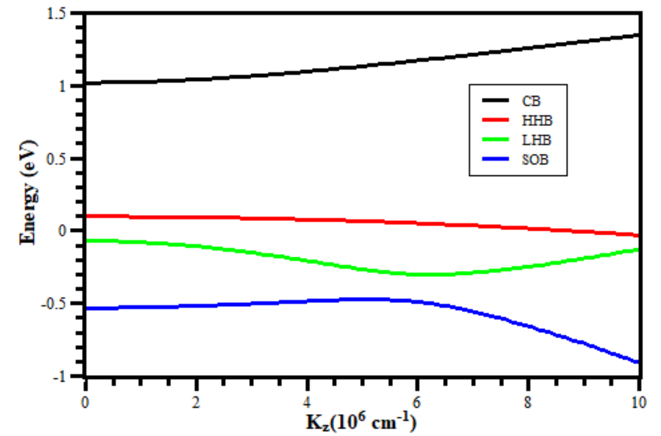

Fig. 2. Band constructions of ternary compound $GaAsSb_0$ /GaAs

The focal structure under examination comprises a p-type InGaAs layer sandwiched between n-type layers of GaAsSb material. With its symmetric energy bandgap, the InGaAs material functions as a quantum well, while the GaAsSb material serves as the barrier layer for charge carriers. The quantum well layer (InGaAs) measures 2 nm in width, while the barrier layer (GaAsSb) spans 4 nm. The entire structure is analyzed on a GaAs substrate at room temperature (300 K). Figure 3 illustrates the energy band diagram for the designed heterostructure.

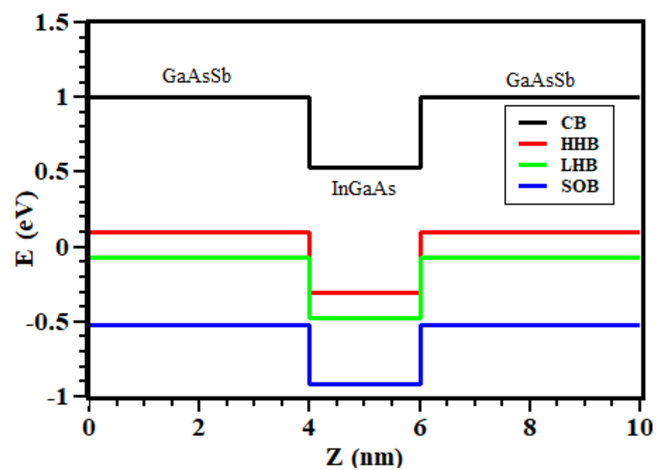

Fig. 3. Energy band diagram of the designed heterostructure

In the process of designing heterostructures tailored for specific applications, the selection of materials and the thickness of layers are pivotal factors influencing the emitted wavelength or radiated energy at the nanoscale level. In this study, the width or thickness of layers (denoted as Z) is meticulously determined through multiple calculations to optimize carrier confinement and effective

recombination of charge carriers. This optimization strategy aims to enhance optical gain at the desired 1550 nm wavelength.

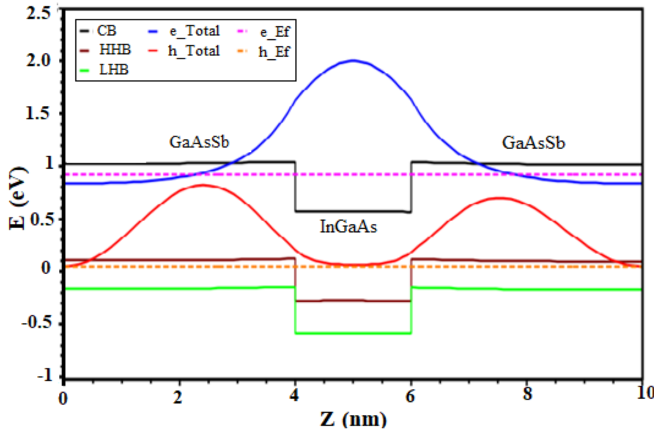

Fig 4. The energy wave function of the designed heterostructure

Analysis of energy wavefunction and band dispersion

The primary objective of this study is to develop a nanoscale heterostructure capable of emitting radiation at a wavelength of 1550 nm with a high optical gain, crucial for enhancing output power. Calculating optical gain necessitates understanding carrier confinement and their distributions. To ascertain carrier localizations, electronic wavefunctions for conduction band electrons and valence band holes are computed. Figure 4 illustrates the calculated wavefunctions for electrons (e_total) and holes (h_total), along with the electron Fermi energy levels.

In determining the confinement of charge carriers within the barrier and well regions, a 6 × 6 Luttinger-Kohn Hamiltonian with effective mass approximation has been employed. This Hamiltonian accounts for the six-band energy levels of split-off, light, and heavy hole bands, including spin up and down states. Figure 4 elucidates that electrons are predominantly confined within the quantum well material, while holes are confined within the barrier material. Consequently, there is an increase in electron density within the well region, resulting in heightened charge carrier recombination and greater optical gain. Table 1 outlines key parameters of compound semiconductors utilized in this study, including constants $\gamma 1$, $\gamma 2$, and $\gamma 3$, which are Luttinger parameters associated with the effective mass of valence subbands.

Table 1. Compound semiconductor key material parameters at 0 K [12]

Material	Lattice Constant (A)	Band Gap (eV)	Effective mass(m_e/m_0)	γ_1	γ_2	γ_3
GaAs	5.653	1.51	0.067	6.98	2.06	2.93
InAs	6.058	0.41	0.026	20	8.5	9.2
AlAs	5.661	3.09	0.15	3.76	0.82	1.42
AlSb	6.135	2.38	0.14	5.18	1.19	1.97
GaSb	6.095	0.81	0.039	13.4	4.7	6

Analysis of optical gain characteristics

To evaluate the performance of the designed heterostructure in terms of amplification, the optical gain is calculated. Figure 5 illustrates the behavior of the computed optical gain with respect to emitted energy. At a temperature of 300 K, the designed heterostructure demonstrates an optical gain of approximately 6000/cm at a radiation energy of 0.8 Ev. This energy corresponds to a wavelength of 1550 nm when converted from energy to wavelength. Consequently, the analyzed results affirm that the proposed design yields a higher optical gain compared to recently designed heterostructures.

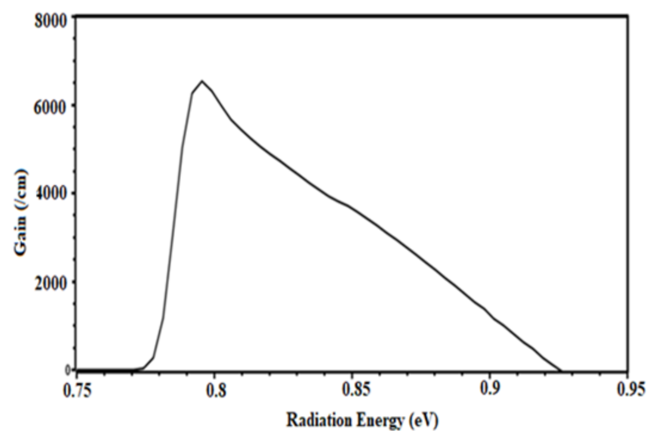

Fig 5: Optical gain characteristics of designed heterostructure

III. RESULTS AND CONCLUSION

this research presents a comprehensive investigation into the design and performance evaluation of a nanoscale heterostructure aimed at emitting radiation with a wavelength of 1550 nm and achieving high optical gain. Through meticulous calculations and analysis, the study demonstrates that the designed heterostructure, consisting of ternary compound materials, exhibits promising characteristics for optoelectronic applications. By employing a 6 × 6 Luttinger-Kohn Hamiltonian and considering carrier confinement, the study reveals favorable carrier distributions, particularly with electrons confined in the quantum well material and holes within the barrier material. This confinement leads to increased carrier recombination and enhanced optical gain, as validated by the calculated energy dispersion profile and optical gain behavior.

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