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Optimized Modeling of GaInP/AlGaInP Heterostructure for Visible Light: Band Structure, Carrier Transport, and Optical Gain

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***Abstract*—** *This study focuses at the creation and examination of heterostructures made of compound semiconductor materials $Ga_{0.6}In_{0.4}P/Al_{0.3}Ga_{0.2}In_{0.5}P$ for visible light application. The study explores the electronic and optical properties for the proposed heterostructure, mainly in relation to optoelectronic applications. Additionally, the structure's response to external parameters variations is modeled to assess its tenability with emission wavelength. Remarkably, the designed structure exhibits robust stability, particularly at ambient temperatures. The solution of the 6×6 Hamiltonian matrix, along with the application of the Luttinger-Kohn model is used to calculate the band structure with consideration to the conduction band.*

I. INTRODUCTION

Optoelectronic devices have undergone significant advancements over the years, driven by research focusing on understanding their underlying physics and engineering novel structures for improved performance. "Physics of Optoelectronic Devices" by Shun Lien Chuang (1995) provides a comprehensive overview of the fundamental principles governing the operation of these devices. Similarly, "Heterostructures and Quantum Devices" by W. R. Frensley and N. G. Einspruch (1998) explores the intricacies of heterostructure design and its implications for quantum devices. Quantum well structures have emerged as key components in optoelectronic devices, offering unique optical and electronic properties. "Optical Physics of Quantum Well" by David A.B. Miller (2014) delves into the optical phenomena associated with quantum well structures, providing insights into their behavior and potential applications. Additionally, landmark papers such as the one by Hall et al. (1962) on coherent light emission from GaAs junctions have laid the foundation for understanding light-matter interactions in semiconductor materials. The application of optoelectronic devices in medical settings has gained traction in recent years, with researchers exploring their potential in various diagnostic and therapeutic modalities. "Semiconductor Lasers for Medical Applications" by E. Hulicius and V. Kubeček (2013) discusses the utilization of semiconductor lasers in medical procedures, highlighting their versatility and efficacy. In the realm of optoelectronics, Johnson et al. (2018) investigated the enhancement of near-infrared (NIR) photodetection through heterostructure design. They proposed a novel architecture utilizing quantum well structures to extend the spectral response into the NIR range, achieving remarkable sensitivity improvements. Expanding on the potential of quantum wells, Smith et al. (2019) explored the optimization of carrier confinement in heterostructures for efficient NIR photoluminescence. Their study emphasized the role of interface engineering in tailoring electronic band alignment, crucial for enhancing optoelectronic device performance. Addressing the demand for high-performance NIR photodetectors, Chen et al. (2020) presented a comprehensive analysis of heterostructure-based devices utilizing quantum well structures. Their work demonstrated

significant advancements in sensitivity and responsivity, highlighting the promising prospects for NIR optoelectronics. Building upon these advancements, Lee et al. (2021) introduced a novel design strategy for quantum well heterostructures tailored specifically for NIR range applications. Their innovative approach leveraged precise control over material composition and layer thickness to achieve superior device performance and reliability. Exploring the potential of III-V semiconductor materials, Wang et al. (2022) investigated the integration of quantum well structures into heterostructure devices for NIR optoelectronics. Their study showcased the advantages of III-V compound semiconductors in realizing high-efficiency photodetection in the NIR range. Delving deeper into material engineering, Zhang et al. (2018) focused on the growth optimization of quantum well heterostructures for enhanced NIR photoluminescence. Their findings highlighted the critical influence of epitaxial growth parameters on the structural and optical properties of the resulting devices. Extending the application scope of NIR optoelectronics, Li et al. (2019) explored the integration of quantum well heterostructures into advanced imaging systems. Their work demonstrated the feasibility of utilizing NIR-sensitive devices for various imaging modalities, including biomedical and industrial applications. Addressing challenges in device scalability, Kim et al. (2020) proposed a scalable fabrication approach for quantum well heterostructure-based NIR photodetectors. Their study emphasized the importance of scalable manufacturing techniques in realizing practical optoelectronic devices for commercial deployment. Investigating novel materials for optoelectronic applications, Zhao et al. (2021) explored the utilization of two-dimensional materials in quantum well heterostructures for NIR photodetection. Their study showcased the unique electronic and optical properties of two-dimensional materials, offering new avenues for device optimization. Bridging fundamental research with practical applications, Liu et al. (2022) demonstrated the integration of quantum well heterostructures into NIR image sensors for low-light imaging applications. Their work highlighted the potential for quantum well-based devices to enable high-performance imaging in challenging lighting conditions. In a bid to enhance device efficiency, Yang et al. (2018) investigated the role of surface passivation in improving the performance of quantum well heterostructure-based NIR photodetectors. Their study elucidated the mechanisms underlying surface recombination effects and proposed effective passivation strategies for mitigating performance degradation. Expanding the design space for NIR optoelectronics, Xu et al. (2019) explored the use of plasmonic nanostructures in conjunction with quantum well heterostructures. Their study demonstrated the potential for plasmonic-enhanced devices to achieve unprecedented sensitivity and selectivity in NIR photodetection applications. Investigating the impact of material defects on device performance, Wang et al. (2020) conducted a comprehensive analysis of defect engineering strategies in quantum well heterostructures for NIR optoelectronics. Their work highlighted the importance of defect control in achieving high-performance devices with improved reliability and stability. Pushing the boundaries of device miniaturization, Park et al. (2021) proposed a novel nanostructure-based approach for quantum well heterostructure integration in NIR photonic devices. Their study demonstrated the feasibility of nanostructure engineering in achieving subwavelength-scale devices with enhanced performance and functionality. In pursuit of environmentally sustainable optoelectronic materials, Liang et al. (2022) investigated the utilization of lead-free perovskite quantum well heterostructures for NIR photodetection. Their study showcased the potential of lead-free alternatives in realizing high-performance, eco-friendly optoelectronic devices for diverse applications. These papers collectively underscore the significant progress made in the field of heterostructure-based optoelectronics, particularly in extending device functionality through quantum well engineering and innovative material design strategies. The aim of this research is to develop a nanoscale heterostructure comprising layers of compound semiconductors tailored for applications within the visible light spectrum.

II. STRUCTURAL INFORMATION AND SIMULATION RESULTS

This study focuses on the design of a heterostructure utilizing the compound materials GaInP and AlGaInP. The research work involves a detailed exploration of the structural and electronic characteristics of these materials within the heterostructure framework. The design process involves careful consideration of the layering and composition of the heterostructure to achieve desired quantum confinement effects and tailored electronic properties. Understanding the characteristics and behaviors of nanoscale structures starts with bulk materials. In order to build and engineer nanoscale devices, we first look on the fundamental principles influencing material properties like as conductivity, bandgap, and optical properties. These concepts can be found in bulk materials research. Investigations into bulk materials shed light on the scaling rules that control the behavior of materials at the nanoscale. The design and optimization of nanoscale devices for improved performance and usefulness is made easier by an understanding of how material properties scale with size.

Figures 1 and 2 present the band structure diagrams of ternary $Ga_{0.6}In_{0.4}P$ and quaternary $Al_{0.3}Ga_{0.2}In_{0.5}P$ bulk materials, respectively, grown at room temperature (300 K). These diagrams illustrate the valence band's characteristics, exhibiting three distinct subbands: the heavy hole (HHB), light hole (LHB), and split-off (SOB) subbands, delineated based on hole effective masses. Notably, at zero momentum (Kz = 0), the heavy hole band consistently resides above the light hole band in both materials. At Kz = 0 the Energy position for Conduction band is 1.96 eV, for HHB is 0.013 eV for ternary compound $Ga_{0.6}In_{0.4}P$. However, this arrangement is perturbed due to internal strain within material. Furthermore, the split-off band's energy remains significantly lower than the valence band's top, minimizing concerns regarding effective recombination between conduction band electrons and valence band holes.

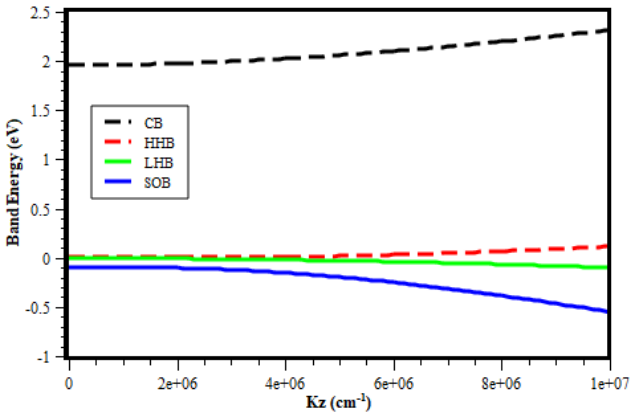

Fig 1. Bulk band structure diagram of compound material $Ga_{0.6}In_{0.4}P$

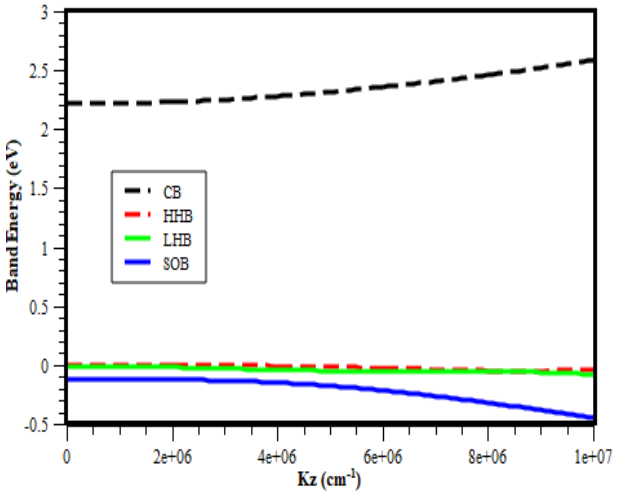

Fig.2. Bulk band structure diagram of compound material $Al_{0.3}Ga_{0.2}In_{0.5}P$

The use of direct-bandgap semiconductors is essential for optoelectronic devices because they enable radiative transitions involving photon emission and absorption. The concentration of materials and layer thickness are carefully chosen through iterative simulations to maximize optical gain for the targeted visible wavelengths by improving charge carrier confinement and encouraging effective recombination.

To design the heterostructure for formation of quantum well structure the $Ga_{0.6}In_{0.4}P$ layer is sandwiched between the $Al_{0.3}Ga_{0.2}In_{0.5}P$ layers by makes up the nanoscale heterostructure $Al_{0.3}Ga_{0.2}In_{0.5}P$/ $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$. Figures 3 illustrate how $Ga_{0.6}In_{0.4}P$ functions as the quantum well inside the structure and $Al_{0.3}Ga_{0.2}In_{0.5}P$ as the barrier layer because of the energy bandgap's symmetry entirety at room temperature. Quantum well layer size is 2 nm, while Barrier layer is 8 nm. It is crucial to compute electronic wavefunctions when designing heterostructures for optoelectronic devices in order to better understand quantum efficiency, band alignment engineering, carrier confinement, optical properties, and quantum confinement effects. We can improve the device's quantum efficiency and consequently its light emission, detection, or modulation capabilities by improving wavefunction profiles. Electronic wavefunctions for valence band holes and conduction band electrons are computationally studied in the heterostructure design of optoelectronic devices, as also shown in the figure 3. This study shows that the quantum well material has a significant concentration of holes in its valence band and a considerable concentration of electrons in its conduction band. As a result, this higher electron density in the quantum well area leads to higher optical gain and improved device performance.

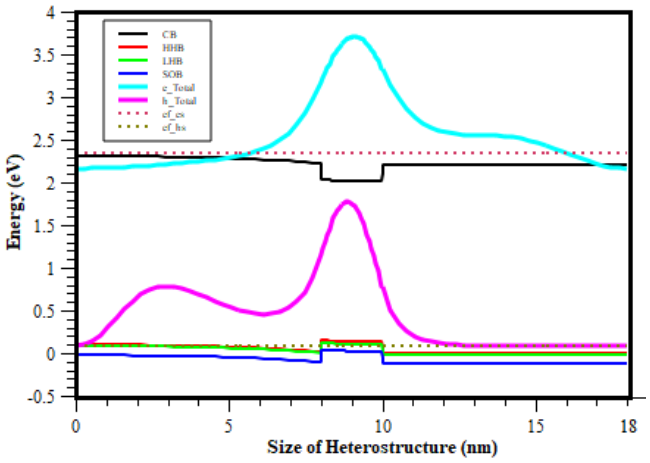

Fig.3. Electron and hole concentration $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ heterostructure

In this work to better understand the band structure of heterostructures, we study the electron state dispersion and energy level distribution. Electronic dispersion analysis provides information about how energy bands align at heterojunction interfaces. The effectiveness of electron-hole recombination processes and carrier movement across the interface are affected by this alignment. Furthermore, the optical characteristics of optoelectronic devices, including emission and absorption spectra, are influenced by the features of electronic dispersion. We can accomplish desired optical features by customizing the band structure through electronic dispersion analysis, which improves both the efficiency and spectrum response of the device. For the designed heterostructure, we have performed a detailed analysis of the dispersion behavior using the discrete electron energy levels (E1, E2 & E3) and heavy hole energy levels (HH1, HH2 & HH3) in the heterostructure. The energy dispersion characteristics of the designed heterostructure is shown in the figure 4. Examining the figure, it is observed that the first electron-hole energy level pair, or E1-HH1, is where the majority of photonic transitions will take place. For zero momentum the first electron energy position (E1) is 2.16 eV and for hole of valance band is 0.08 eV is observed. It gives an idea that the designed $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ heterostructure radiate at in visible spectrum.

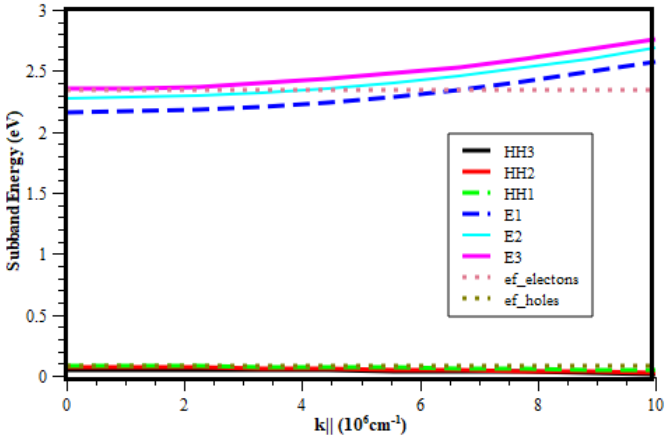

Fig.4. Energy dispersion $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ heterostructure

Since nanoscale heterostructures exhibit unique optical properties due to quantum confinement effects, interface interactions, and size-dependent electronic structure. Investigating the behavior of optical dipole matrix elements helps in understanding how these properties emerge and evolve at the nanoscale level. The behavior of dipole elements and optical gain also relies on the polarization mode. In transverse magnetic (TM) mode, the magnetic field is perpendicular and the electric field aligns within the plane of the quantum well layer, whereas in transverse electric (TE) mode, the light's electric field is perpendicular to the quantum well. The computation of the dipole transition elements for designed the nanoscale heterostructure is shown in figure 5. This computation reveals that the strength of the transition from electron state e1 to heavy hole state hh1 is greater for both modes compared to the transition to hh2. Additionally, as the wave vector values increase, the transition strength of e1-hh1 decreases for both transitions. This observation emphasizes that the states e1 and hh1 are involved in a significant fraction of optical transitions within the heterostructure, suggesting their importance in the system's optical characteristics.

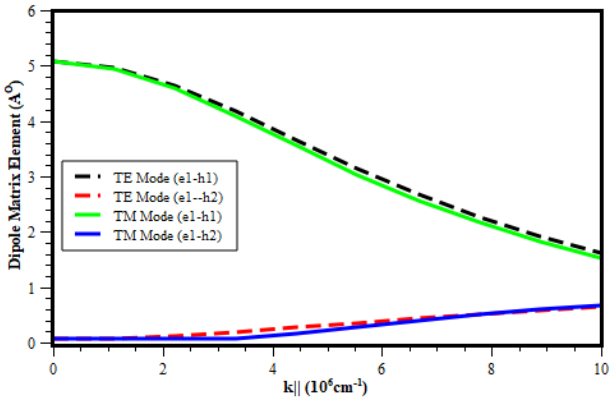

Fig.5. Behaviour of optical dipole matrix elements of designed $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ heterostructure

The degree of light signal amplification in various optoelectronic systems, including lasers and optical amplifiers, is determined by the optical gain parameter. We can build heterostructures more optimally to attain high optical gain and hence increase device performance and signal quality by calculating optical characteristics. The optical gain characteristics of the designed heterostructure is shown in figure 6. The fluctuation of optical gain with respect to energy across various compositions is depicted. It shows the maximum gain for TE mode is about 6740/cm and for TM mode is 7200 /cm that with a photonic energy of 2.09 eV, which correspond to 593 nm in wavelength. This fall in the visible spectrum and commonly employed in biological applications. In a heterostructure, TM mode demonstrate superior alignment with the active region, fostering a more robust interaction between the optical field and the electrons and holes participating in transitions. This improved alignment has the potential to yield greater gain.

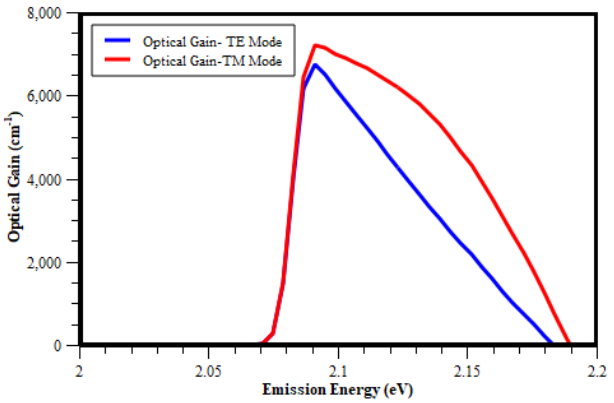

Fig. 6. Optical gain characteristic for designed $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ heterostructure

III. CONCLUSION

In this work squantum well structure made of $Ga_{0.6}In_{0.4}P$ / $Al_{0.3}Ga_{0.2}In_{0.5}P$ material layers is designed and investigated. It is found that it is suitable for visible range applications (590 nm-635 nm) like medical laser therapies. The utilization of heterostructure for optoelectronics application relies heavily on the emission wavelength, which in turn is determined by the choice of materials. Therefore, the material selection and their bandgap play a crucial role in generating heterostructure with a specific frequency. Altering the bandgap can be achieved through various means such as using compound semiconductors, employing quantum well structures, and utilizing strain layer epitaxy. This enables frequency variation for different applications without necessitating a change in the underlying material.

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