



An Investigation into Temperature-Dependent Optical Properties of InGaAsP/InP Nanoscale Heterostructures

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Abstract

The present study has undertaken a theoretical investigation into the temperature-dependent optical properties and Lasing Characteristics of an $\text{In}_{0.69}\text{Ga}_{0.31}\text{As}_{0.56}\text{P}_{0.44}/\text{InP}$ nanoscale heterostructure, with specific focus on the role of the anti-guiding factor in determining material gain and its variation with carrier density. The study also examined how differential gain and refractive index respond to changes in carrier concentration. Material gain spectra for transverse electric (TE) modes were simulated and analysed as functions of wavelength and photon energy. The influence of temperature on the optical behaviour of the heterostructure has revealed distinct changes under varying thermal conditions. The results of temperature dependence of the anti-guiding factor and differential gain have highlighted the potential of this nano-heterostructure for future nano-optoelectronic applications.

Keywords: Optical Properties, Material Gain, Anti-Guiding Factor, Nano-Heterostructure.

1. Introduction

Recent researches on quantum-sized structures based III–V semiconductors have gathered worth mentioning interest owing to their distinctive physical and electronic properties [1– 55]. It is found that the self-assembly of low-dimensional semiconductor layers allows three-dimensional electron confinement within coherent, dislocation-free clusters [7–8]. Researchers have reported that reducing threshold current, enhancing optical gain and minimising losses are critical parameters for quantum well (QW) based lasing heterostructures. Further, step-based separate confinement heterostructures (SCH) effectively confine carriers within the quantum well, increasing carrier density and promoting radiative recombination process, thereby improving device efficiency [9–11]. These quantum-sized heterostructures are very crucial for modern optoelectronic applications such as fiber-optic communications, optical data storage, and remote sensing, offering advantages like continuous-wave operation, low heat generation, and reduced power consumption [12–13]. However, the optical and electronic properties of materials like InGaAs are found to be highly temperature-dependent, with elevated temperatures typically causing redshifts and reduced optical gain due to changes in non-linear absorption and thermal conductivity [12–13]. Growth temperature also influences structural parameters [14–16]. Numerous researches on nano-scale heterostructures including quantum dots, wires, and wells have been carried out for their potential in advanced optoelectronic technologies [17–18]. Among these, it is revealed that type-I and type-II QW heterostructures have promise for laser diodes and quantum cascade lasers (QCLs) [19]. While type-I QWs are restricted to emission wavelengths shorter~3.7 μm , type-II QWs offer extended wavelength operation, making them suitable for long-wavelength applications [20]. Their tunability through band offset engineering and strain application further enhances their versatility [21]. Recent research studies on InGaAs/GaAsSb type-II heterostructures have delineated high optical gain in the short-wave infrared (SWIR) region [22–23]. Similarly, interband cascade lasers (ICLs) based on type-II InAs/GaInSb QWs have attained mid-infrared (MIR) emission. M-shaped type-II InAs/GaSb and GaAsSb/InGaAs super lattices have

been efficiently utilised in mid and long-wavelength infrared detectors and lasers, with room-temperature emission around $2.41\ \mu\text{m}$ [22–23]. It is noteworthy to mention over here that Ryczko and Sęk proposed a broken-gap M-shaped type-II QW structure using GaInSb/InAs for ICLs targeting MIR emission. Besides these advancements, achieving efficient high-temperature or room-temperature operation in III–V semiconductor-based heterostructures remains a dynamic area of research [24–37]. For example, Fuchs et al. delineated high-temperature lasing in W-shaped type-II (GaIn) As/Ga (AsSb)/(GaIn)As QWs at 1200 nm and 1300 nm. The review studies have emphasised the growing interest in type-II quantum heterostructures based on III–V direct band gap materials such as InAs/GaSb [24–25], InP/GaAs [26], GaSb/GaAs [27–28], GaAs/GaAsSb [29–30], InAs/AlSb [31], InAlAs/InP [32–33], and InGaP/InP [34–35]. These structures provide enhanced flexibility in band gap and extended infrared emission, making them ideal for IR optoelectronic devices. The study reveals the influence of temperature on optical gain characteristics as a function of wavelength and photonic energy, revealing distinct behaviours higher than ambient temperature and lower than ambient temperature [37]. The $k\cdot p$ method (a powerful theoretical approach) has been used to calculate the electronic band structure of semiconductors [38]. In view of the above, the present study aims to examine the temperature-dependent optical properties of $\text{In}_{0.69}\text{Ga}_{0.31}\text{As}_{0.56}\text{P}_{0.44}/\text{InP}$ nanoscale heterostructure using the $k\cdot p$ method. The analysis yields insights into carrier dynamics, band structure modifications, and optical gain behaviour under varying thermal conditions, thereby contributing to the design of efficient infrared optoelectronic devices.

2. Structural and Theoretical Details

The proposed $\text{In}_{0.69}\text{Ga}_{0.31}\text{As}_{0.56}\text{P}_{0.44}/\text{InP}$ nanoscale heterostructure comprises a quantum well of InGaAs with a thickness of $60\ \text{\AA}$, sandwiched between InGaAsP barrier layers and enclosed by InP cladding. The details of structural parameters are mentioned in the Table 1.

Table 1: Details of structural parameters for InGaAsP/InP nanoscale heterostructures

InP	Cladding ($100\text{\AA}$)
$\text{In}_{0.69}\text{Ga}_{0.31}\text{As}_{0.56}\text{P}_{0.44}$	Barrier($60\text{\AA}$)
$\text{In}_{0.49}\text{Ga}_{0.51}\text{As}$	QW($60\text{\AA}$) Active Region
$\text{In}_{0.69}\text{Ga}_{0.31}\text{As}_{0.56}\text{P}_{0.44}$	Barrier($60\text{\AA}$)
InP	Cladding($100\text{\AA}$)
InP	Substrate

The entire structure is designed to be fabricated on an InP substrate, selected for its favourable material properties. InP is a direct band gap semiconductor with a zinc blende crystal structure, widely recognised for its application in optoelectronic devices and optical fiber systems [39–40]. It offers high electron velocity, greater electron mobility, and reduced parasitic effects, contributing to lower noise levels, in particular at high frequencies. Moreover, its high dielectric constant and inherent resistivity make it a superb electrical substrate and offers natural isolation. In such nano-heterostructures, the presence of the gain mechanism together with the resonant cavity enables it perceived phenomenon [39–40]. Among several characteristics, the material gain allied with different polarisation modes (Table 1) is significantly crucial. The material gain arises from the processes of light generation and the recombination of electrons and holes for the step separate confinement lasing nano-heterostructures (Fig.1). The material gain as a function of energy can be simulated using the following model:

$$G(E') = \frac{q^2 M_B^2}{E' c \hbar \epsilon_0 n_{eff} m_0^2} \sum_{i,j} \int_{E_g}^{E_{gb}} m_{r,ij} c_{ij} A_{ij} (f_c - f_v) L(E) dE,$$

Where q denotes charge, M_B represents the bulk momentum transition matrix element, ϵ_0 refers to free space permittivity, c is the velocity of light, n_{eff} indicates the effective refractive index, W corresponds to the width of the quantum well, i, j are the conduction and valence band quantum numbers, $m_{r,ij}$ signifies the spatially weighted reduced mass for transition, c_{ij} expresses the spatial overlap factor between the states i and j , A_{ij} describes the angular anisotropy factor, f_c and f_v denote the electron quasi Fermi function in the conduction and valence band and $L(E)$ stands for the Lorentzian lines shape function.

In addition, the temperature dependent of material gain, can be expressed as

$$G(E) = \frac{\pi \hbar e^2}{n E c \epsilon_0 m_0^2} [1 - e^{(E - \Delta f / K_B T)}] \sum_{n_c, n_v} \frac{|M|^2}{4\pi^2 L_w} f_c f_v \frac{\frac{\hbar}{\tau}}{\pi (E_{eh} - E)^2 + (\frac{\hbar}{\tau})^2} dk_x dk_y,$$

Where Δf denotes the quasi Fermi level separation, E represents the photonic energy, K_B refers to the Boltzmann constant, m_0 signifies the effective mass of electron in free space, e indicates the charge of electron, T corresponds to temperature, ϵ_0 stands for the free space permittivity, n denotes the refractive index, c is the velocity of light, $|M|^2$ expresses the squared optical transition matrix element of momentum for transition between n_v and n_c , n_v is the hole sub bands, n_c is the electron sub bands, $\hbar$ represents reduced plank constant, f_c denotes the Fermi-Dirac distributions for electrons in the conduction bands, f_v denotes the Fermi-Dirac distributions for holes in the valence bands and τ signifies the intra band relaxation time. Next, vital factor is the anti-guiding factor that depicts a significant and decisive role in analysing the material gain of the heterostructure. This factor can be specified in terms of differential gain and change in refractive index as

$$\alpha = \frac{4\pi(-\frac{dn}{dN})}{\lambda(\frac{dG}{dN})}$$

where the quantities dn/dN and dG/dN are the differential refractive index and differential gain respectively for the heterostructure [40].

Refractive index and carrier concentration in reference to the effective band gap [46] is specified as $\mu = \mu(E) = (A + \frac{B}{[1 - C^2(E'/1.237)^2]})^{1/2}$, where A , B and C are the constants, E' is the modified photonic energy specified as

$E' = E_{GO} - \frac{1}{3}(F_c + F_v)$, where F_c and F_v are the respective quasi Fermi levels for electrons & holes in conduction and valence bands [43-44]. Thus, if carrier concentrations are known, then refractive index can be simply computed.

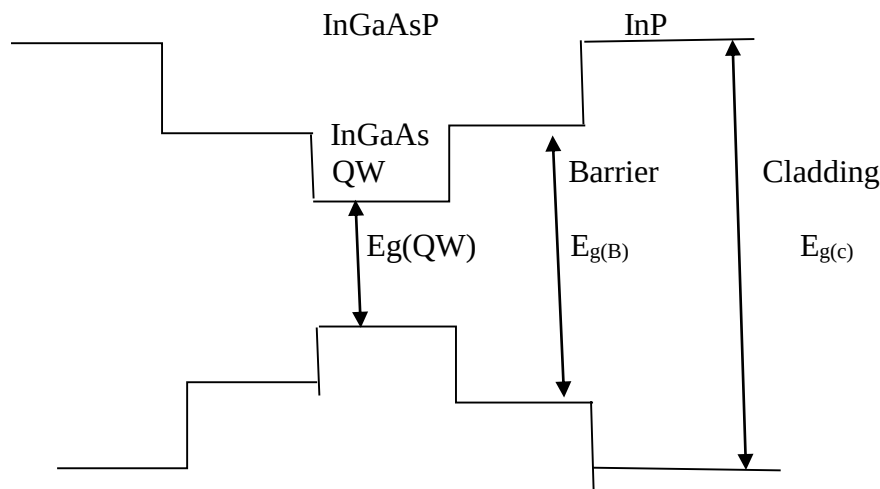


Figure.1: InGaAs /InP nano heterostructure (a) Energy- band diagram [48].

3. Results and Discussion

The anti-guiding factor plays a significant function in the research investigations pertaining to lasing characteristics of nano-heterostructures. This factor is influenced by the differential gain and refractive index of the structure. Therefore, understanding the behaviour of differential gain is essential. It can be calculated by differentiating the material gain with regard to the carrier density. It is revealed that differential gain decreases exponentially as carrier density increases in regard to InGaAs/InP nano-heterostructure. Further, the effect of temperature on differential gain has been computed and its behaviour is depicted in Figure 2:

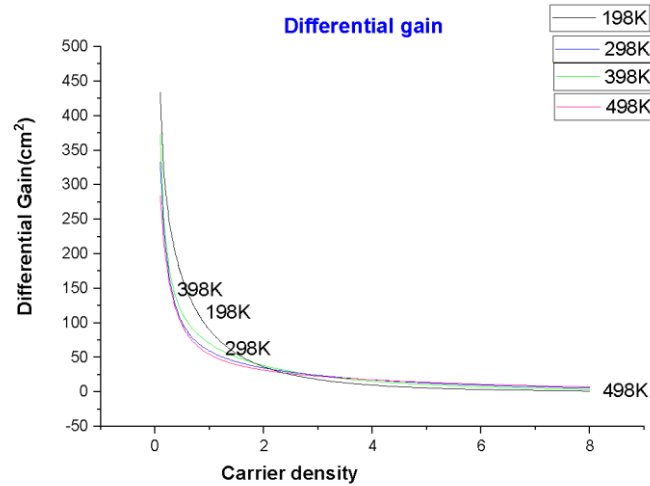


Figure 2: Temperature dependence of differential gain with carrier density (in cm^{-3}).

As can be noted from Figure 2 that there is a notable variation in the curvature of differential gain plot, when plotted under different temperature conditions. Figure 2 clearly depicts an exponential decrease over the temperatures range from 100K to 500K with a downward shift in peak differential corresponding to the temperature increase. This is in agreement with the earlier research [47]. Figure 3 depicts the plot of anti-guiding factor versus current density for $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ lasing nano-heterostructure at different temperatures. It is evident from the Figure 3 that the anti-guiding factor increases as the current density increases for $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ lasing nano-heterostructure. Compared to differential gain, the anti-guiding factor influences the material gain behaviour of the $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ nano-heterostructure. Its simulated results for the anti-guiding factor align with earlier researches.

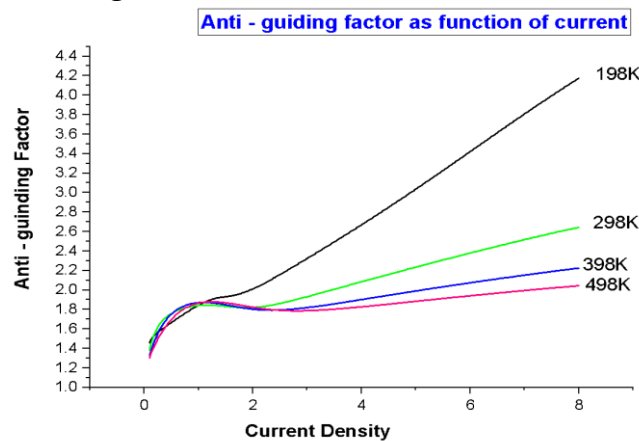


Figure 3: Variation of anti-guiding factor with current density (in A/cm^2) at different temperatures.

It has been reported that the values of anti-guiding factor for lasing nano-heterostructures at ambient temperature vary typically 2.0-6.22. However, in the proposed design, these values vary 1.0 -3.0 at ambient temperature. It is worthwhile to mention over here that large values of the anti-guiding factor can be influential in inducing anti-guiding effects in narrow band lasing nano-heterostructures and self-focusing and filamentation in broad area emitters [48]. An epitaxial structure designed with a low optical confinement factor and less sensitive to filamentation have been reported [5] and confirmed by a number of analyses of single pass tapered region amplifiers and simple analytical models. Furthermore, the variation of the anti-guiding factor with current density has also been conducted at different temperatures and its variation is depicted in Figure 3. The analysis revealed that, as the temperature increases, the range of the anti-guiding factor decreases, enabling the nano-heterostructure to function effectively even at higher temperatures.

Afterward, the temperature dependent of material gain of $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ lasing nano-heterostructure has been simulated with regard to wavelength and photonic energy. Their respective spectra at different temperatures are plotted in Figures 4 and 5. The information evoked from the material gain simulations specify that the behaviour of material gain as a function of lasing wavelength and photonic energy is noteworthy at different temperatures. Plots of material gain with varying wavelength and photon energy at different temperatures (Fig. 4 and 5) have depicted a minimal increase in material gain at the lasing wavelength of $0.82\mu\text{m}$ and the photonic energy of 1.50 eV. The aforementioned discussion stimulates the relevance of proposed $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ nano-heterostructure under both conditions of low and high temperatures for the opto-electronic applications.

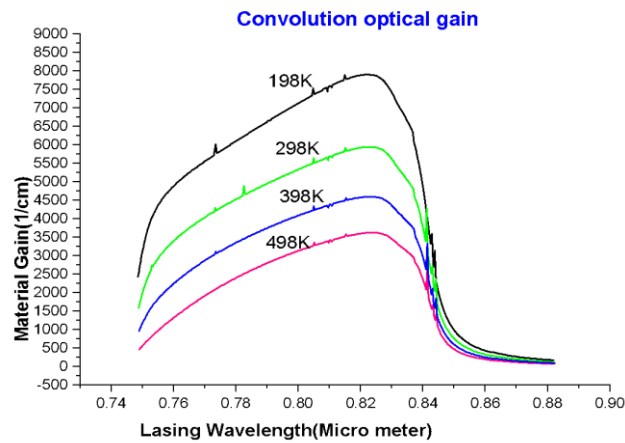


Figure 4: Material gain with lasing wavelength (in μm) at different Temperatures.

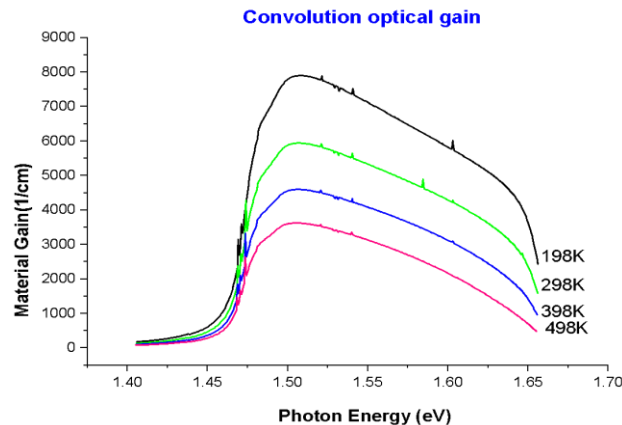


Figure 5: Material gain with photonic energy at different temperatures.

An important, though sometimes challenging, feature of lasing nano-heterostructures is their sensitivity to carrier-induced variations in the refractive index of the active layer. This feature proves primarily noteworthy when designing optical waveguides, as variations in carrier density can significantly change the refractive index profile. The primary cause of this behaviour often arises from the band gap difference between the two semiconductors forming the heterostructure, which enables spatial confinement of the injected carriers. Such confinement augments optical gain but also introduces refractive index modulation that need to be carefully managed. Moreover, temperature has a deceive role in influencing carrier dynamics and refractive index changes.

The temperature-dependent of carrier-induced refractive index is depicted in Figure 6, revealing its impact on device performance across different operating conditions [49– 50]. Figure 6 illustrates that the carrier-induced refractive index changes increasingly negative as the temperature raises, indicating a stronger impact on device performance at elevated functioning conditions.

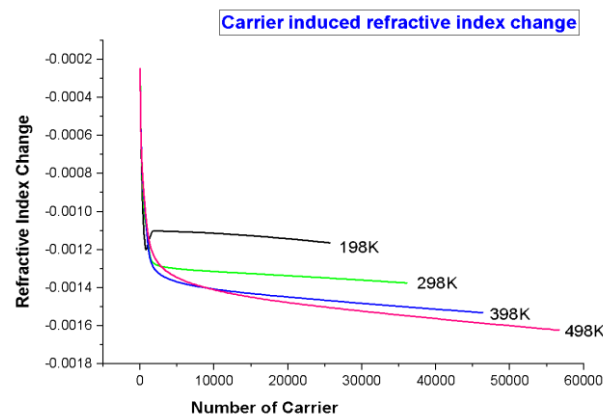


Figure 6: Temperature dependence of refractive index change with number of carrier.

4. Conclusion

It is concluded from the findings of the present study that the temperature-dependent optical properties of InGaAsP/InP nanoscale heterostructures exhibit promising lasing characteristics in the proposed $\text{In}_{0.49}\text{Ga}_{0.51}\text{As}/\text{InP}$ nano-heterostructure. It is revealed from the analysis of the anti-guiding factor, differential gain and refractive index that they greatly influence the lasing characteristics and optical properties of the nano-heterostructure. Analysis of material gain with varying wavelength and photon energy at different temperatures has delineated that there is a minimal increase in material gain at the lasing wavelength of $0.82\mu\text{m}$ and the corresponding photonic energy of 1.50 eV and the structure exhibits distinct behaviour under low and high conditions of temperatures. In particular, the material gain increases as temperature decreases at a fixed lasing wavelength, consistent with reduced carrier scattering and enhanced optical transition probability at lower temperatures. Besides, the findings of this study support the suitability of the proposed structure for operation across a wide temperature range and highlight its prospects for advanced nano-optoelectronic applications.

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