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Transparent level temperature dependence of semiconductor lasers

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Abstract

The point at which a material stops being absorptive is called transparency. Gain in the active medium of a laser device cannot occur unless the carrier concentration exceeds the transparency density. If the semiconductor is further pumped beyond transparency by optical or electrical means, the gain becomes equal to the total loss and the material starts to lase at the threshold level. Joule heating, free carrier absorption, and band filling effects change the refractive index of the semiconductor and hence the lasing wavelength. The change of the refractive index with temperature is referred to as the thermo-optic effect. This work presents a semi-classical numerical model to investigate the temperature dependence of the carrier concentration, operating voltage, and refractive index at transparency level for GaAs, $In_{0.15}Ga_{0.85}As$, and $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$ over the temperature range from ≈ 20 ^{o}K to ≈ 400 ^{o}K. Results revealed that the transparency lasing wavelength fit with temperature obeys a rational equation. In addition, the refractive index change due to band filling is calculated at transparency over the studied temperature range and modeled as third order polynomial in temperature. The study concludes that there is a material-dependent temperature at which the band to band transition contribution to the refractive index is minimum and found to be ≅ 186.6 ^{o}K, ≅ 252 ^{o}K, and ≅ 298 ^{o}K for GaAs, $In_{0.15}Ga_{0.85}As$, and $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ in order. The refractive index change due to free carriers was found to be more sensitive to temperature variation than the refractive index change due to band to band transition.

Keywords: transparency wavelength, refractive index change, $In_{(1-x)}Ga_xAs_yP_{(1-y)}$

INTRODUCTION

The development of modern society is based mainly on the ability to communicate information. Among the approaches in this direction, there exist semiconductor laser diodes for use as modulation sources in optical communication links. The major force behind research into semiconductor laser is to obtain more powerful and faster communication links. Lasers are also used extensively in many areas of science as a research tool and in industrial application (Ling et al., 2020). Semiconductor lasers are particularly significant because of their compact size, lower threshold current, and higher efficiency compared with other types of lasers (Ling et al., 2019; Struckmeier and León, 2019). The transparent carriers, threshold current density and the gain are important characteristics of laser diodes which define the possibility of their practical use and affect all the basic parameters. Stimulated emission can only occur when the occupation probability of electrons in the conduction band f_c exceeds the occupation probability of electrons in the valence band f_v. This condition is equivalent to Bernard and Duraffourg's inequality

$$\mu_c - \mu_v > \hbar\omega \tag{1}$$

where μ_c and μ_v are the quasiFermi energy, respectively, and $\hbar\omega$ is the incident photon energy. Both the gain and absorption are zero when the incident photon energy is smaller than the lowest possible transition energy -the band gap energy. When the incident photon energy is greater than the difference in quasiFermi levels, Bernard-Burafforg's relation is violated and the medium becomes absorptive. The medium is also absorptive when $\mu_c - \mu_v > \hbar\omega$. Hence, gain is produced for photon energies

$$E_g < \hbar\omega < (\mu_c - \mu_v) \tag{2}$$

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In the context of laser physics, the medium becomes transparent when the rate of upward transition from the valence band to the conduction band equal to the rate of downward transition. In this case, there would be no loss or gain. Specifically, we are referring to transparency at the lasing energy, i.e., the photon energy corresponig to the maximum of the the gain spectrum.
III-V compounds are the most common semiconductor materials used in diode laser fabrication. The lattice matching relation of $In_{(1-x)}Ga_xAs_yP_{(1-y)}$ to InP is

$$x = \frac{0.189y}{0.4176-0.0125y} \qquad 0 < y < 1.0 \tag{3}$$

where x and y are the composition fractions. The relation gives the end point $x = y = 0$ for InP and $y = 1.0$, x = 0.468 for $In_{0.532}Ga_{0.468}As$ (Adachi, 1992).

The variation of the refractive index with temperature play an important role in optoelectronic devices, fiber optics as well as biological and chemical analysis (Della Corte et al., 2000; Zhao et al., 2019). Key parameters such as the threshold current, wavelength and efficiency depend on the device temperature. The refractive index is usually divided into a constant term (temperature independent) and a temperature dependent term arising from phonon-phonon interactions (Guo et al., 2015). The thermo-optic coefficient is a measure of the change of the refractive index with temperature. It is defined as the derivative of the refractive index with respect to temperature. There are two main factors which alter the refractive index i) variation due to carrier injection and ii) variation due to change in the temperature.

The thermo-optic effect was investigated experimentally and theoretically for specific spectral range in various places (Guo et al., 2015; Wang et al., 2014; Zhao et al., 2019). The modified single oscillator model is a semi-empirical method used widely to determine the room temperature refractive index of a large class of III-V semiconductors (Melati et al., 2016). However, little is known about the variation of the refractive index with temperature due to the free carrier effect and the banding filling effect. The objective of this work is to study how the operating voltage, lasing wavelength as well as the change in the refractive index due to free carriers and band filling vary with temperature at transparency for some common III-V compounds.

MODEL USED IN THE CALCULATIONS

Within the semiclassical theory, the laser field is treated classically while the material medium is calculated using quantum statistical mechanics. The charge neutrality condition is a constrain on the gain medium. It states that the total number of electrons in the conduction band must be equal to the total number of empty states in the valence band (Blood, 2015). Mathematically,

$$\int_{E_g}^{\infty} g_{cv}(E_{ba})[f_c(E_{ba}) + f_c(E_{ba}) - 1]\, dE_{ba} \tag{4}$$

where $g_{cv}(E_{ba}) = (2m_cm_v/(m_c + m_v))^{\frac{3}{2}}(2\pi^2\hbar^3)^{-1}\sqrt{E_{ba} - E_g}$ is the joint density of states; m_c is the effective mass of an electron in the conduction band and m_v is the effective mass of an electron in the valence band, i.e., equivalently a hole. The electron occupation probabilities in the conduction and valence bands are given, respectively, by

$$f_c(E_{ba}) = \frac{1}{1 + exp\,\{[m_v\frac{E_{ba}-E_g}{m_c+m_v} - \mu_c + E_c]/kT\}} \tag{5}$$

$$f_v(E_{ba}) = \frac{1}{1 + \exp\,\{[-m_c\frac{E_{ba}-E_g}{m_c+m_v} - \mu_v + E_v]/kT\}} \tag{6}$$

Using Eq. (4) and the injection potential V_{op}, the quasiFermi levels can be determined. Within the free carrier model, the linear gain coefficient was shown in various places –see for example (Yamada, 2014) – to be given by

$$g = \frac{\hbar\omega}{\varepsilon_0 n_r \tau_d}\int_{E_g}^{\infty}\frac{|\mu_{ba}|^2 g_{cv}(E_{ba})[f_c(E_{ba}) - f_v(E_{ba})]}{(\hbar\omega - E_{ba})^2 + (\hbar/\tau_d)^2}dE_{ba} \tag{7}$$

Taking into consideration the spin-orbit interaction Δ . The dipole moment spectral dependence is taken as

$$|\mu_{ba}|^2 = \left(\frac{q^2}{6m_0\omega_{ba}}\right)\left(\frac{m_0}{m_c} - 1\right)\frac{E_g(E_g + \Delta)}{E_g + 2\Delta/3} \tag{8}$$

Electronic transition, Joule heating and free carrier effects are the three basic physical processes that determine the optical properties of materials (Weber, 2002) . The intensive injection of carriers changes the interband absorption (Paskov and Pavlov, 1992). When the states in the bottom of the conduction band are filled, electrons in the valence band are optically excited to energies in the conduction band higher than the nominal band gap. This is explained by the band filling effect. Variation in the

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carrier concentration shift the refractive index due to the bandgap filling, bandgap shrinkage and plasma effects (Bennett et al., 1990). It is very complicated to determine all the factors which affect the refractive index of a semiconductor. However, the dominant part of the refractive index which is independent of the injected carriers is caused by bound electrons or deeply located electrons. Another part is caused by free carrier absorption within the same band (plasma effects). The contribution to the total refractive index change due to band to band transition is (Yamada, 2014)

$$\Delta n_b = \frac{1}{2\varepsilon_0 n_r}\int_{E_g}^{\infty} \frac{|\mu_{ba}|^2 g_{cv}(E_{ba})[f_c(E_{ba}) - f_v(E_{ba})](\hbar\omega - E_{ba})}{(\hbar\omega - E_{ba})^2 + (\hbar/\tau_d)^2} dE_{ba} \tag{9}$$

The change of the band gap due to temperature can be found from Varshni's equation (Varshni, 1967)

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta} \tag{10}$$

The fitting parameter α and β in case of $In_{0.15}Ga_{0.85}As$ are slightly different from the values of GaAs. However, we use the following relation for $In_{0.15}Ga_{0.85}As$, and $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ (Kuo et al., 2007)

$$E_g(T) = 1.347 - 0.788y + 0.149y^2 - 4.1 \times 10^{-4}\left[\frac{T^2}{T+\alpha} - \frac{\beta^2}{\beta+\alpha}\right] \tag{11}$$

Various parameters needed in the gain calculations are summarized in Table 1.

Table 1: Material parameters for the semiconductors used in this study

Parameter name	Symbol	GaAs[a]	$In_{0.15}Ga_{0.85}As$[b]	$In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$[c]	Units
Band gap at 0^oK	$E_g(0)$	1.519	1.3031	0.84	eV
Band gap offset	Δ	0.34	0.062	0.326	eV
Electron effective mass	m_c/m_0	0.08	0.05569	0.0449	--
Heavy hole effective mass	m_v/m_0	0.5	0.4865	0.438	--
Refractive index	n_r	3.6	3.3948	3.514	--
Fitting parameter	α	5.4×10^{-4}	5.7×10^{-4}	136	$eV/{}^{\circ}K$
Fitting parameter	β	204	249	300	$^{\circ}K$
Dephasing time	τ_d	10^{-13}	10^{-13}	10^{-13}	s
Nonradiative lifetime	τ_s	10^{-9}	10^{-9}	10^{-9}	s

[e]extracted from (Ahmed and Yamada, 1998; Varshni, 1967) [b]extracted from (Holly et al., 2013) [c]extracted from (Goldberg and Schmidt, 1999)

RESULTS AND DISCUSSION

Gain is dominated by the product of density of states and $f_c - f_v$, which represent the degree of inversion. The former depends mainly on the effective masses and the square root of the transition energy measured with respect to the band gap. Gain is produced only for energies around the band gap. Larger proportions of the injected carriers contribute to the gain at low temperature compared with their contribution at room temperature. At constant carrier concentration, the gain diminishes with raising temperature, Fig.1 (a). The gain curve is broadened due to depolarization and scattering. It should be note that the slowly decaying tails of the Lorentz line shape function leads to photon absorption at energies below the band gap energy. The Lorentzian function is empirically replaced by $\sec\left(\frac{E_{ba}-\hbar\omega}{\hbar/\tau_d}\right)$ with faster decaying tails (Chow and Koch, 1999). At a specific temperature, as the carrier concentration increases, the gain peak rises and the lasing wavelength is blue shifted because of the band filling effect, Fig.1 (b). The dependence of the material absorption edge on the carrier concentration is generally known as the Burstein-Moss effect (Burstein, 1954). This phenomenon has been explained by the band filling effect. When the states in the conduction band are filled to an appreciable extent, the apparent band gap of the semiconductor increases because of pushing the absorption edge to higher energy. Hence, exciting electrons from the valence band to the conduction band require energies greater than the nominal band gap (Bennett et al., 1990). Since holes in the valence band has a large effective mass and hence a larger density of states, the band filling effect for them is small. Once the linear gain has been calculated, the linear gain peak can be found. The next stage is to vary the injected carriers and repeat the procedure for a range of temperatures --from 20 $^{\circ}K$ to 400 $^{\circ}K$ in this study. All the calculations in this work were done on Wolfram Mathematica.

Transparency occurs at the points of zero gain shown in Fig.1 (c). The transparent carrier density $N_{tr}(T)$ was reported to vary with $T^{\frac{3}{2}}$ (Sale, 1993)

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$$N_{tr}(T) = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}(m_c m_v)^{\frac{3}{4}} \tag{12}$$

The best fit to the data is, however, a vertically shifted exponential growth as seen in Fig.2 (a) according to

$$N_{tr}(T) = A_0 e^{T/T_{tr}} - N_0 \tag{13}$$

where A_0, T_{tr}, and N_0 are material dependent fitting parameters−listed in Table 2. Oscillation is a state where there is output without input. The threshold gain is the optical gain required to sustain laser oscillations. It is equal to the total loss in the cavity, i.e., the internal loss plus the mirror loss. This condition dictates that there is a minimum carrier concentration for continuous laser oscillations called the threshold carrier concentration. It follows that the threshold carrier concentration is

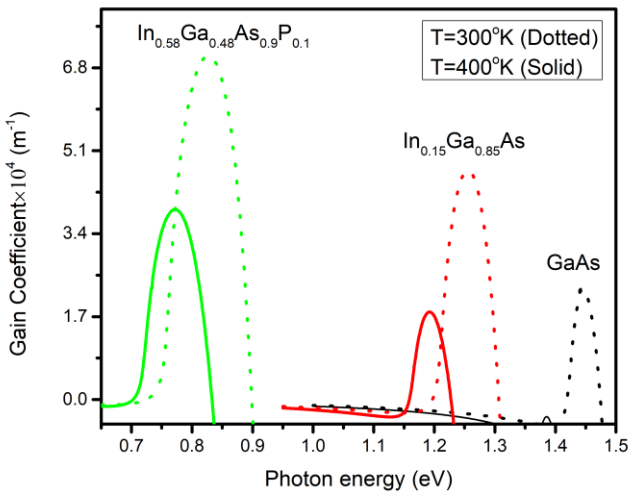
$$N_{th}(T) = \frac{1}{\Gamma_a v_g a \tau_{ph}} + N_{tr}(T) \tag{14}$$

$$= \frac{1}{\Gamma_a v_g a \tau_{ph}} + \left(A_0 e^{T/T_{tr}} - N_0\right) \tag{15}$$

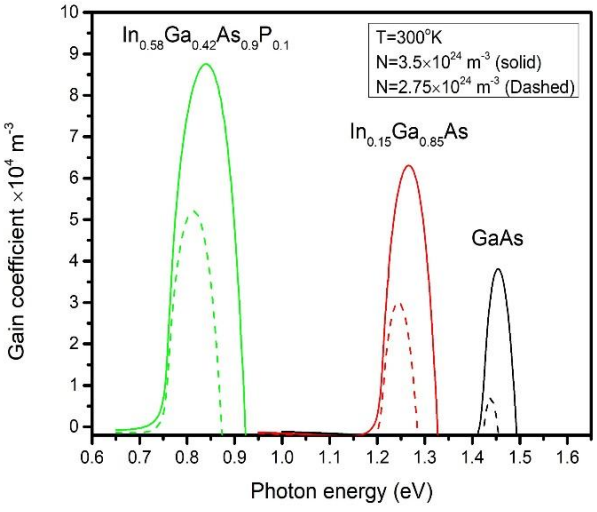
where Γ_a, v_g, a, τ_{ph} are the confinement factor, group velocity, gain cross section and photon lifetime in the active layer, respectively. The active layer has length $= 250\ \mu m$, width $= 2\ \mu m$ and thickness $= 0.2\ \mu m$ (Agrawal and Dutta, 2013). To get the threshold current multiply the threshold concentration by the volume and elementary charge and divide that by the carrier lifetime. As Fig.1 (d) shows, the threshold current of $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ is around $9.4\ mA$ followed by $In_{0.15}Ga_{0.85}As$, $\approx 12.6\ mA$, and GaAs, $\approx 17.3\ mA$. The low value of $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ threshold current is attributed lasing at long wavelength $\lambda = 1.55\ \mu m$. Consequently, it has a lower power slope coefficient compared with the other two material which lase at shorter wavelengths. Small values of the threshold current are favorable for laser operation. According to Eq. (12), light electrons and holes leads to low threshold current (Numai, 2015).

Table 2: Transparent carrier concentration fitting-parameters

Material	A_0 (m^{-3})	T_{tr} $(°K)$	N_0 (m^{-3})	*Adj. R-square*
GaAs	4.647×10^{24}	777.513	4.583×10^{24}	0.99947
$In_{0.15}Ga_{0.85}As$	3.324×10^{24}	786.059	3.252×10^{24}	0.99976
$In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$	3.586×10^{24}	1059.413	3.569×10^{24}	0.99914

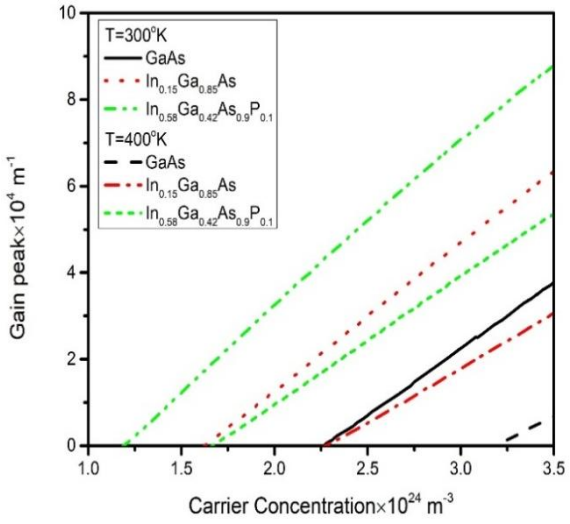


(a)

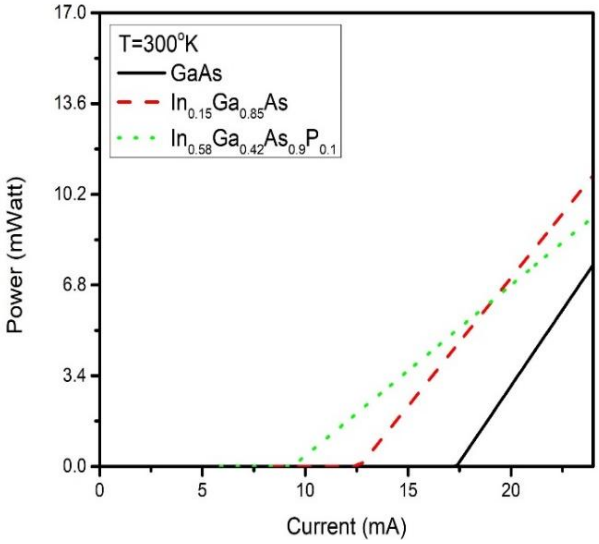


(b)

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(c)



(d)

Fig. 1: (a) Linear gain for $300°K$ and $400°K$ and carrier concentration $N = 3 \times 10^{24}\ m^{-3}$ (b) Linear gain for two different carrier concentration (c) Gain peak variation with carrier concentration (d) Output optical power

In addition, transparency is achieved in GaAs at higher carrier concentration than $In_{0.15}Ga_{0.85}As$ and further lower values in $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$ at any temperature−Fig.2 (a). The behavior is characterized by the fit temperature T_{tr}. This result can be understood as the transparency operating voltage of $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ is lower than $In_{0.15}Ga_{0.85}As$ and GaAs at all temperatures. At transparency, the operating voltage temperature dependence profile is similar to the profile of the band gap as shown in Fig.2 (b). The following equation describes how the operating voltages depends on temperature at the transparent level

$$V_{op}(T) = V_0 + b_0 T + c_0 T^2 + d_0 T^3 \qquad measured\ in\ eV \tag{16}$$

where the fitting parameters V_0, b_0, c_0, and d_0 are listed in Table 3. It follows that the transparency wavelength can be expressed as

$$\lambda_{tr}(T) = \frac{2\pi\hbar c}{qV_{op}(T)} \tag{17}$$

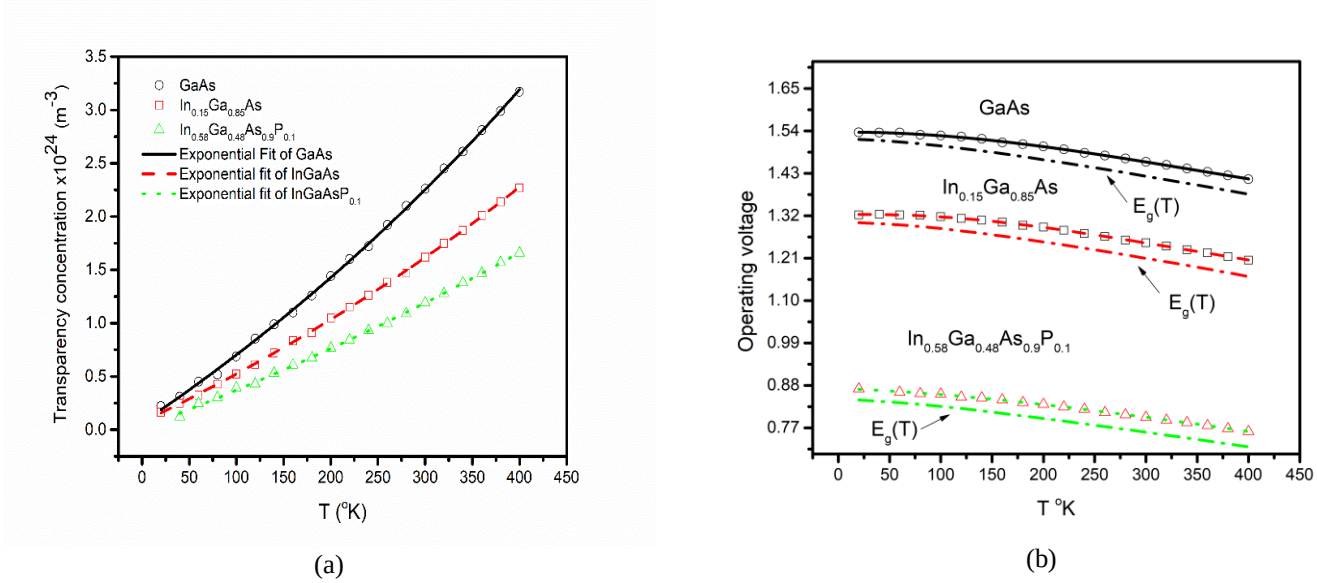
$$= \frac{\lambda_0}{1 + \frac{b_0}{V_0}T + \frac{c_0}{V_0}T^2 + \frac{d_0}{V_0}T^3} \tag{18}$$

$\hbar$, c, q are the reduced plank's constant, speed of light in vacuum and the elementary charge, respectively. $\lambda_0 = \frac{2\pi\hbar c}{qV_0}$ is the transparency wavelength at $T = 0°K$.

Table 3: The Operating voltage fitting parameters at transparency

Material	V_0 eV	b_0 $(eV/°K)$	c_0 $(eV/°K^2)$	d_0 $(eV/°K^3)$	*Adj. R-square*
GaAs	1.537	3.185×10^{-5}	-1.346×10^{-6}	1.279×10^{-9}	0.99924
$In_{0.15}Ga_{0.85}As$	1.322	9.833×10^{-5}	-1.620×10^{-6}	1.620×10^{-9}	0.99956
$In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$	0.8722	-1.004×10^{-4}	-6.438×10^{-7}	4.956×10^{-10}	0.99912

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(a) (b)

Fig. 2: (a) Transparency concentration dependence with temperature (b) Variation of the transparency operating voltage with temperature

Most of the heat generated in the active region of a laser diode is due to nonradiative recombination. Increasing the injection current leads to raising the temperature of lasing medium in a process called resistive heating or Joule's heating, as well (Butt et al., 2020). The heating induced refractive index is proportional to the temperature change (Numai, 2015)

$$\Delta n_T = (2\sim5) \times 10^{-4}\, \Delta T \tag{19}$$

where ΔT is the change in temperature in Kelvin. Since this effect increases the refractive index of the active region, the confinement of light is enhanced.

Free carriers interact with the lattice and undergo transition within the same band. The plasma effect is modeled as being proportional to carrier concentration (Bennett et al., 1990)

$$\Delta n_c = -\frac{q^2}{2m^*\omega^2\varepsilon_0 n_r}\, N \tag{20}$$

here, m^* is the effective mass of the free carriers. Evidently, the plasma contribution decreases with the square of the photon energy. The net result is antiguiding of light and a reduction in the refractive index. At carrier concentration $\sim 10^{24}\ m^{-3}$, Δn_c is in the order of 10^{-3}. At transparency, $N \longrightarrow N_{tr}$. Substituting Eq. (13) into Eq. (20) yields the free carriers refractive index change as a function of T at transparency

$$\Delta n_c = -\frac{q^2}{2m^*\omega^2\varepsilon_0 n_r}\, (A_0 e^{T/T_{tr}} - N_0) \tag{21}$$

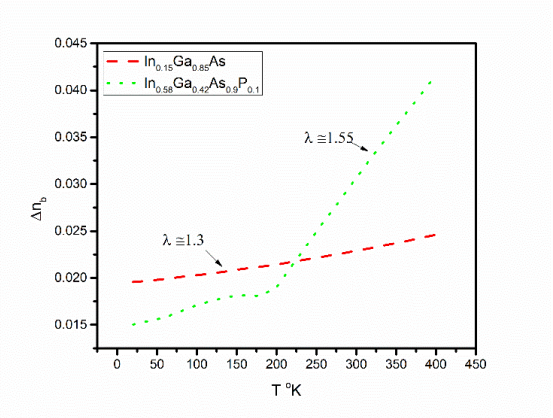
$\frac{d\Delta n_c}{dT}$ represents the contribution of the free carrier to thermo-optic coefficient. At $T = 300°K$ and $\lambda = 1.3\ \mu m$, $\frac{d\Delta n_c}{dT}$ is $-2.86 \times 10^{-5}\ °K^{-1}$ for GaAs, $-2.70 \times 10^{-5}\ °K^{-1}$ for $In_{0.15}Ga_{0.85}As$, and $-3.18 \times 10^{-5}\ °K^{-1}$ for $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$.

The refractive index change due to band filling is shown in Fig.3 (a) at the wavelengths of minimum loss in fiber optics for $In_{0.15}Ga_{0.85}As$ and $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$ that emit light at 1.3 and 1.55 μm respectively.

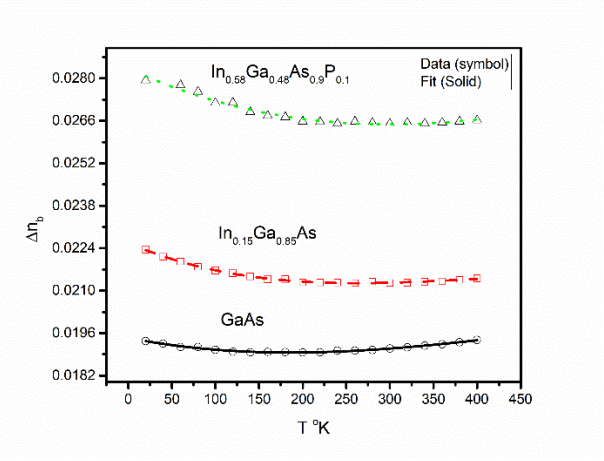
Table 4: Refractive index change fitting parameters at transparency

Material	*A*	*B*	*C*	*D*	*Adj. R-square*
GaAs	0.01944	-5.615×10^{-6}	1.863×10^{-8}	-1.270×10^{-11}	0.9877
$In_{0.15}Ga_{0.85}As$	0.02257	-1.216×10^{-5}	3.524×10^{-8}	-3.059×10^{-11}	0.99549
$In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$	0.02832	-1.324×10^{-5}	2.684×10^{-8}	-1.049×10^{-11}	0.96701

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(a)



(b)

Fig. 3: Refractive index change versus temperature for $In_{0.15}Ga_{0.85}As$ (dash lines) and $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$ (dotted lines) (b) Refractive index change at transparency

This part contribution to the refractive index of $In_{0.15}Ga_{0.85}As$ is almost proportional to the temperature at $\lambda = 1.3\ \mu m$. However, its variation in case of $In_{0.48}Ga_{0.58}As_{0.9}P_{0.1}$ at the spectral wavelength of $\lambda = 1.55\ \mu m$ is much more complicated. The band to band refractive index change at transparency can be expressed as a cubic function in temperature

$$\Delta n_b = A + BT + CT^2 + DT^3 \tag{22}$$

where the fit parameters A, B, C, and D are listed in Table 4. This effect is on the order of $\sim 10^{-2}$ at $T = 300°K$. The band filling induced refractive index decrease with temperature till a minimum value is reached after which the behavior is reversed – Fig.3 (b). The temperature at which the minimum value occurs is $T \approx 186.6°K$, $\approx 252°K$ and $\approx 298°K$ for GaAs, $In_{0.15}Ga_{0.85}As$ and $In_{0.58}Ga_{0.42}As_{0.9}P_{0.1}$ in order. At $T = 300°K$, $\frac{d\Delta n_b}{dT}$ is in the order of $\sim 10^{-6}$ for the three materials.

CONCLUDING REMARKS

In this work, the carrier density, operating voltage, and lasing wavelength have been calculated as a function of temperature at transparency. As T tends to zero, the transparency densities of the three materials approach as small as values in the orders of $10^{22}\ m^{-3}$. The transparency wavelength red shifts as the temperature increases. The band-to-band refractive index change as a function of temperature looks like a parabola where the vertex locates the point of minimum contribution to the wavelength shift. As the temperature varies, the refractive index change due to free carriers is altered at a higher rate compared with the refractive index change associated with band filling.

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