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Numerical Study on the Optical Properties of III-V Quaternary Compounds Aluminium Gallium Indium Phosphide Light Emitting Diode

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Abstract

The research works the quaternary compounds of AlGaInP (Aluminum Gallium Indium Phosphide) LEDs that provide luminescence intensity in high-brightness LEDs. AlGaInP LEDs, which are direct bandgap semiconductors with green color emission and a wavelength ranging from 500 to 565 nm, are important in electronics display and liquid crystal backlight applications. Depend on carrier concentration, the desired colors and luminescence intensity, the mole fraction of the quaternary compound is changed and also the bandgap energy. The paper contributions the carrier distribution of holes and electrons, the density of states, and the fermi-dirac distribution function calculated. Based on the carrier concentration, luminescence intensity versus photon energy has been determined. These simulation results are presented using MATLAB simulation with theoretical approach.

A. Introduction

Nowadays, light-emitting diodes play crucial roles in modern society and semiconductor device technology, especially an LED, can convert electrical energy into optical energy. AlGaInP (aluminum gallium indium phosphide) is a semiconductor material used in optoelectronic devices, such as light-emitting diodes (LEDs) and laser diodes [1].

AlGaInP (LEDs) have important applications in automotive signal lighting, automotive interior lighting, traffic signal lights, large area display, and liquid crystal display backlighting. AlGaInP are determined by the energy band structure of the material, which is influenced by the composition and alloying of aluminum (Al), gallium (Ga), indium (In), and phosphorus (P).

The bandgap energy generally ranges from about 1.9 to 2.4 electron volts (eV), which corresponds to the visible spectrum of light. The AlGaInP-based devices can be controlled by adjusting the aluminum content (Al composition) in the alloy and a direct bandgap semiconductor material when the aluminum composition, x, is smaller than 0.53, corresponding to an emitting wavelength about 532 nm has been reported by M.an-Fang Huang et.al [2]. In optoelectronic devices, the material system used determines the output power and the wavelength of the device. AlGaInP LEDs have the visible range (green, yellow and orange which means that a high proportion of the injected electrons and holes get recombined and generated photons. There are many semiconductor binaries, such as GaAs and InP, have high efficiency. The ternaries and quaternaries made of two or three binaries, such as AlP, InP and GaP, showed good efficiency over a good range of composition [9].

The main challenges of the quaternary compound (AlGaInP) LED, the desired colors and luminescence intensity, the composition(x) of the ternary compound is changed based on carrier concentration. The research system is to get the carrier (electron in CB, hole in VB) distribution of AlGaInP. The semiconductor of the material III-V quaternary alloys is formed by the two mixing ternary compounds that are composed up of two group-III and two group-V elements. Sadao Adachi reviewed the basic semiconductors of III-V ternary and quaternary compounds based on an interpolation scheme are described [3-8].

Section II shows density of states and the fermi-dirac distribution function, the concentration of hole in the valence band, electrons concentration in the CB and luminescence intensity versus photon energy are investigated. Section III and IV describe the simulation results and conclusion. Figure1 shows the implementation procedure is described by step by step.

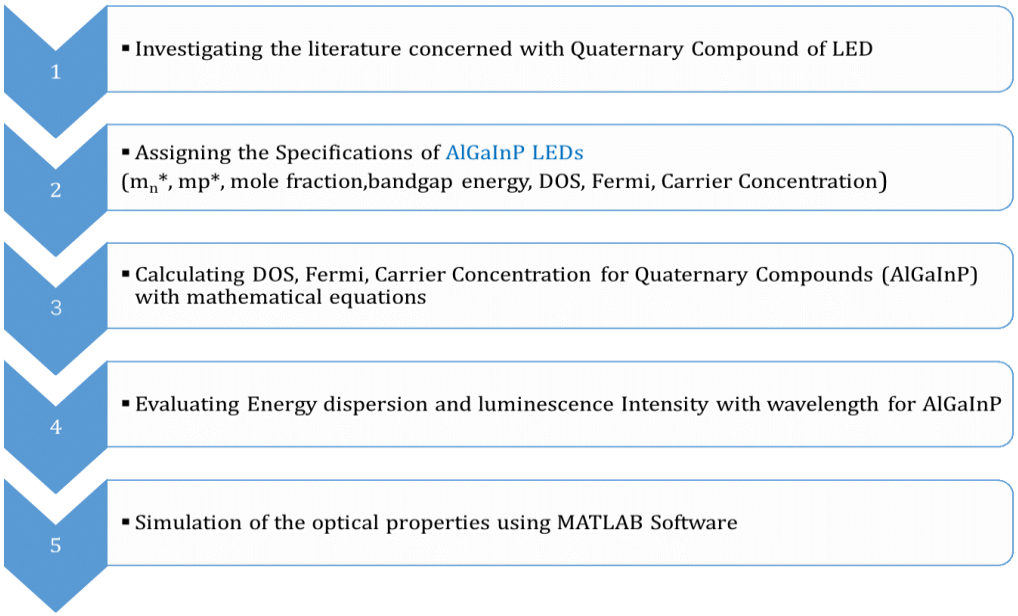

Figure 1. Implementation Procedure

B. Materials and Reserach Methods

The composition of ($Al_xGa_yIn_{1-x-y}P$) varied by adjusting the ratios of aluminum, gallium, indium, and phosphorus. By changing the composition, it is possible to tune the material's bandgap, which determines the wavelength of light that the compound can emit or absorb. The bandgap energy of $Al_xGa_yIn_{1-x-y}P$ is between 1.9 eV and 2.4 eV. In Quaternary Compounds, the composition varied from 0 to 1, x is the composition of aluminum alloy,1-x is the composition of gallium alloy, and 1-x - y is the composition of indium alloy[10].

The quaternary compounds of the band gap energy, various composition (mole fractions), and bowing factors of these alloys. These parameters are usually referred to as the specifications of AlGaInP LED described in Table 1.

Table 1. Specifications of AlGaInP

No	Materials	*AlGaInP*
1	m_n^*	$0.04m_0$
2	m_p^*	$0.56m_0$
3	h	6.625×10^{-34}JS
4	hbar	1.054×10^{-34}JS
5	k	1.38×10^{-23}J/K
6	Eg at 300K	2.32 eV
7	kT	25.86meV
8	C	3×10^8m/s
9	Composition of x,y,1-x-y	0.35,0.15,0.5

Density Of States

The states density based on quantum mechanical consideration of vital parameters for carrier concentration are calculated [3,4,6].

$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}, (E \geq E_c) \quad (1)$$

$$g_v(E) = \frac{m_p^* \sqrt{2m_p^*(E_v - E)}}{\pi^2 \hbar^3}, (E \leq E_v) \quad (2)$$

Where,

$g_c(E)$ = conduction band state density at an energy

$g_v(E)$ = valence band state density at an energy

Fermi-Dirac Distribution

The bandgap energy between the two allowed bands single-particle states in a quantum system at zero temperature is called fermi energy [3,4,6]. $(E-E_F) >> kT$, the Fermi probability function is reduced to the Boltzmann approximation for each state that was occupied by electrons, which is described in an equation.

$$f(E) = \exp\left[\frac{-(Ec - E_F)}{kT}\right] \quad (3)$$

For energy states $E < E_v$, If $(E_F-E_v) >> kT$, the probability function is reduced to the Boltzmann approximation, which is described in an equation.

$$1 - f(E) = \exp\left[\frac{-(E_F - E_v)}{kT}\right] \quad (4)$$

Where;

f(E) denotes the probability distribution function

Fermi Energy is abbreviated as E_F

Carrier Concentrations

The concentration of electrons at the conduction band and holes at the valence band are distributed over the empty conduction band and valence band states, respectively, as function of energy. The distribution depends upon the temperature. Therefore, it is important to find the electron and hole distribution over the required energy range, in order to determine the carrier concentration [3],[4]. The carrier concentration of electrons at the CB is the density of allowed quantum states in the CB multiplied by the probability of a state is occupied by an electron [6].

$$n(E) = g_c(E)f(E) \quad (5)$$

$$n = N_c \exp\left(\frac{-(E_c - E_F)}{kT}\right) \quad (6)$$

$$N_C = 2\left[\frac{2\pi m_n^* kT}{h^2}\right]^{\frac{3}{2}} \quad (7)$$

Where;
Nc is the state in which effective density functions in CB.
m_n * is the density of the electron's effective mass in its ground state

Similarly, hole distributions are calculated according to the probability that a state of energy exists, energy levels attained by density are multiplied as follows:

$$p(E) = g_V(E)\left[1 - f(E)\right] \quad (8)$$

$$p = N_V \exp\left(\frac{-(E_F - E_C)}{kT}\right) \quad (9)$$

$$N_V = 2\left[\frac{2\pi m_p^* kT}{h^2}\right]^{\frac{3}{2}} \quad (10)$$

Where;
Nv is the density of effectiveness at valence band edge
mp * is the density of the hole's state effective mass.

Emission Spectrum

The electron–hole pairs (ERP) of spontaneous recombination and the simultaneous emission of photons released by semiconductor LEDs. In semiconductor lasers and super-bright LEDs, there is a difference between the stimulated emission process and the spontaneous emission process [7,8]. Electrons and hole are concerned with the parabolic dispersion are presented by equation.

$$E_c = \left[\frac{\left(E_g q + h^2 k^2\right)}{2m_e}\right] \quad (11)$$

$$E_v = \left[-\frac{h^2 k^2}{2m_h}\right] \quad (12)$$

Emission Intensity

An emission intensity is calculated from the product of the joint density of states and the distribution of carriers in the allowed bands[7,8] which is given by equation:

$$\rho(E) = \frac{1}{2\pi^2}\left[\frac{2m_r^*}{(\frac{h}{2\pi})^2}\right]^{\frac{3}{2}}\sqrt{(E - Eg)} \quad [13]$$

The distribution of carriers in the allowed bands is calculated by the Boltzmann distribution

$$f_B(E) = e^{\left(\frac{-E}{kT}\right)} \quad (14)$$

$$I(E)\alpha\sqrt{(E - E_g)}\exp(\frac{-E}{kT}) \quad (15)$$

The maximum emission intensity occurs at

$$E=E_g+ kT/2 \quad (16)$$

At full width at half maximum,

$$\Delta E \approx 1.8kT \quad (17)$$

C.Results and Discussion

Figure2 describes the theoretical analysis of the AlGaInP LEDs from the mathematical equations and the simulation results of the LED model. The bandgap energy of Al $_x$Ga$_y$In$_{1-x-y}$P is 2.32eV taking into account Vegard law with mole fractions close to Al $_{0.35}$ Ga$_{0.15}$ In$_{0.5}$ P, which is lattice-matched to GaAs.

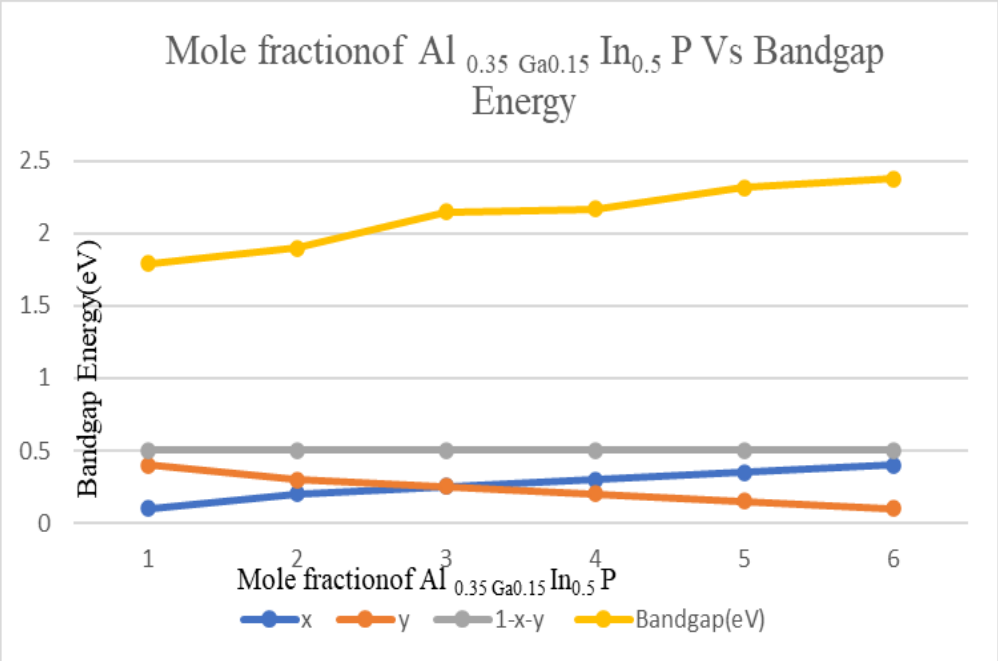

Figure 2. Mole Fraction of Al $_{0.35}$ Ga$_{0.15}$ In$_{0.5}$ P

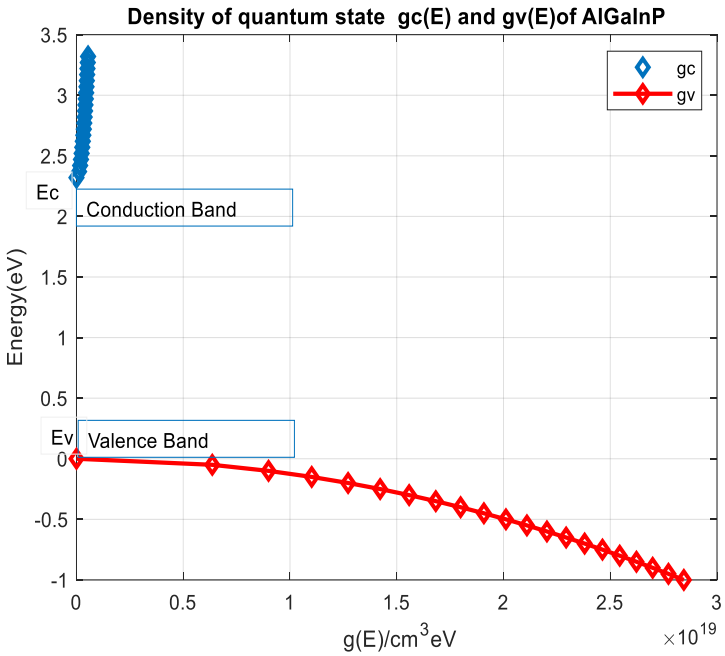

Figure 3. Density of Energy States

Figure3 presents the energy states that are available at each energy in the semiconductor and depending on square root of Energy. Moreover, the states density increasing electron energy moves upwards above in the conduction band whereas the state of hole energy moves downward below the valence band.

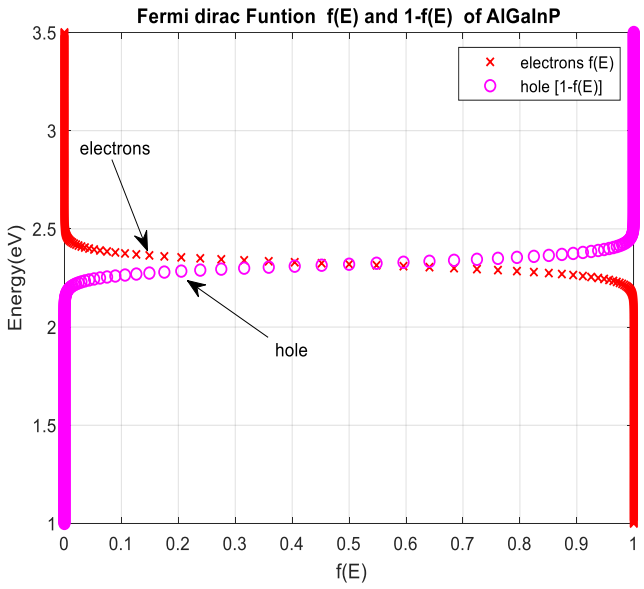

Figure 4. Fermi- Dirac Function

Figure4 exhibits the energy versus Fermi-Dirac function of AlGaInP. The percentage of states are filled by an electron and hole at a given energy.

Figure5 illustrates an electron-hole recombination process in which the semiconductor materials of AlGaInP energy dispersion are accompanied by an energy gap from state to state.

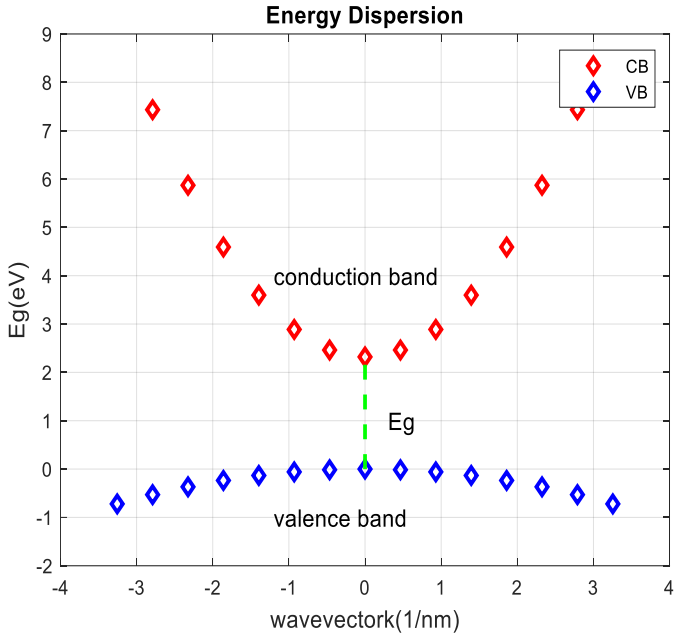

Figure 5. Energy Dispersion

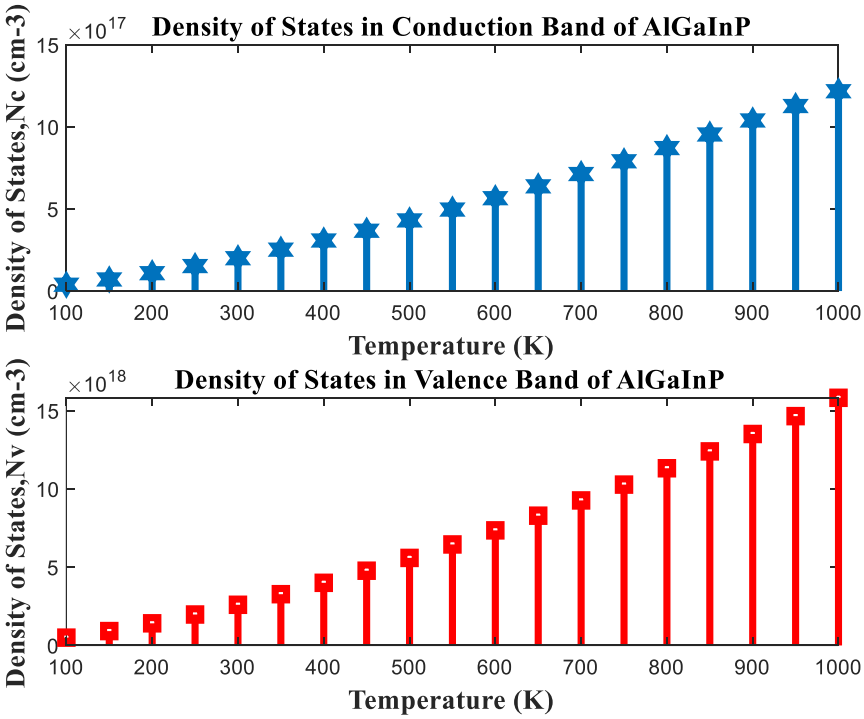

Figure 6. Density of States in Conduction Band and Valence Band of AlGaInP Material

By using equations (7) and (10), the effectiveness of the conduction band density of states ($2\times10^{17}cm^{-3}$) and the effective density corresponding to the top

of valence band ($2.6\times10^{16}cm^{-3}$) respectively.Figure6 points out the density of states at conduction band and valence band of AlGaInP leds depend on the difference temperature.

$$N_C = 2\left[\frac{2\pi m_n^* kT}{h^2}\right]^{\frac{3}{2}}$$

$$N_C = 2\left[\frac{2\pi \times 0.04 \times 9.11\times10^{-31} \times 1.38\times10^{-23}}{(6.626\times10^{-34})^2}\right]^{\frac{3}{2}}$$

$$N_C = 2\times10^{17}\,cm^{-3}$$

$$n = N_C exp\left(\frac{-(E_C - E_F)}{kT}\right)$$

$$= 2\times10^{17}\,cm^{-3}\times0.098$$

$$= 1.96\times10^{16}\,cm^{-3}$$

$$N_v = 2\left[\frac{2\pi m_p^* kT}{h^2}\right]^{\frac{3}{2}}$$

$$N_v = 2\left[\frac{2\pi \times 0.56 \times 9.11\times10^{-31} \times 1.38\times10^{-23}}{(6.626\times10^{-34})^2}\right]^{\frac{3}{2}}$$

$$N_v = 2.6\times10^{18}\,cm^{-3}$$

$$p = N_V exp\left(\frac{-(E_F - E_C)}{kT}\right)$$

$$= 2.6\times10^{18}\,cm^{-3}\times0.91$$

$$= 2.37\times10^{18}\,cm^{-3}$$

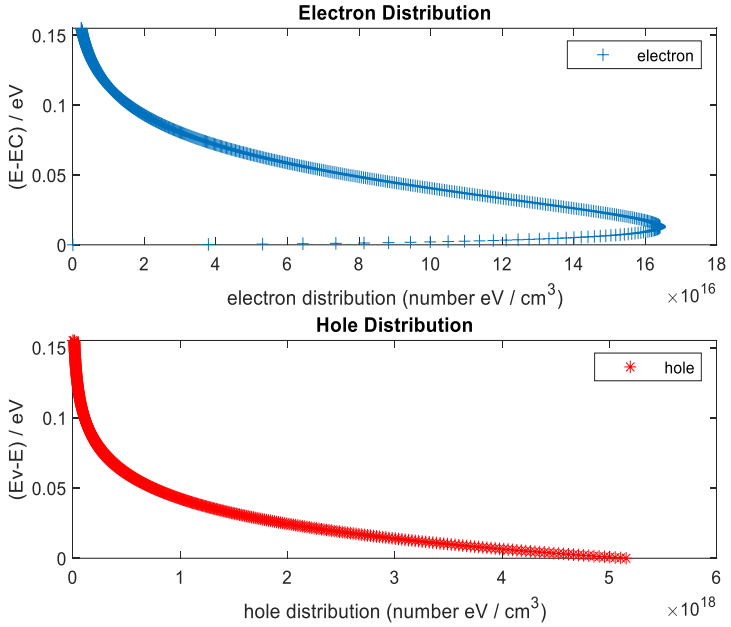

Figure 7. Carrier Concentrations

By using equations (5) and (8), the AlGaInP carrier concentrations of electrons ($1.96\times10^{16}cm^{-3}$) in CB and the carrier concentrations of holes ($2.37\times10^{18}cm^{-3}$) in VB in Figure7.

The peak emission intensity value of AlGaInP is 8.58 lm/sr at photon energies of 2.33 eV. The full wave-half maximum value of this compound is between 2.316 eV and 2.364 eV. The spectral width of the AlGaInP compound is 47 meV and the wavelength range is 531nm.

Figure8 presents emission spectrum based on carrier concentration of AlGaInP. The results showed the luminescence intensity of $Al_{0.35}Ga_{0.15}$ $In_{0.5}$ P based LED degrades significantly for green color emission wavelength 531nm is used for high-brightness LEDs. The color emission wavelength of LED is attained by choosing a specific semiconductor material with bandgap energy.

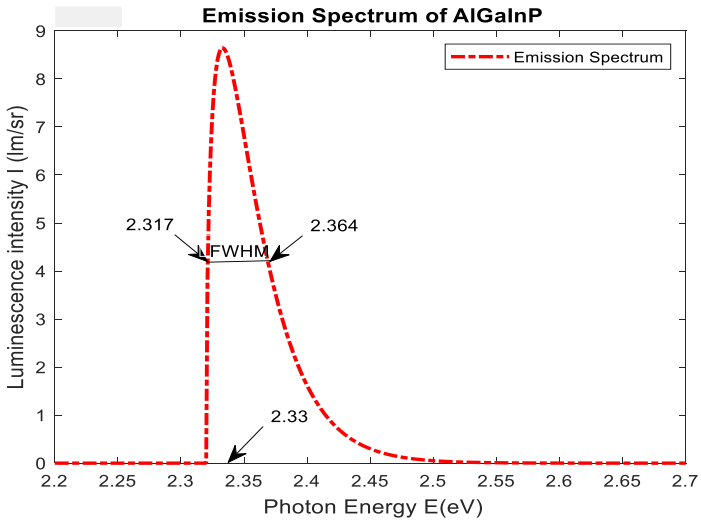

Figure 8. Emission Spectrum based on carrier concentration

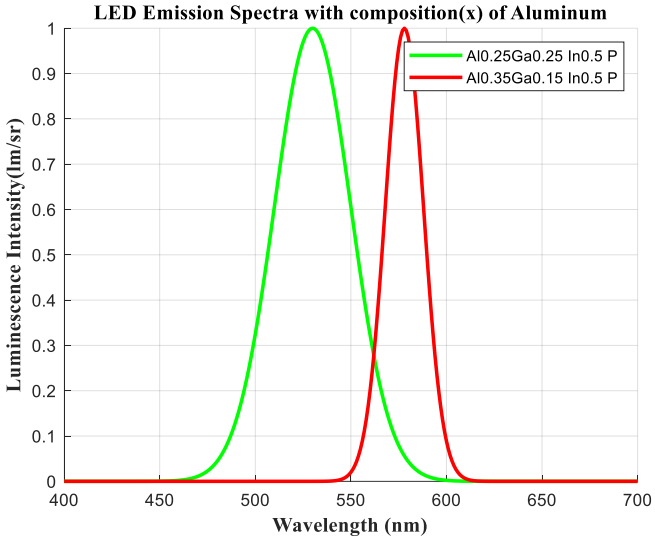

Figure 9. Luminescense Intensity versus Wavelength $Al_{0.35}Ga_{0.15}$ $In_{0.5}$ P**.**

Figure 9 implies the emission spectrum with composition(x) of Aluminum versus luminescence intensity of the $Al_{0.35}Ga_{0.15}$ $In_{0.5}$ P and $Al_{0.25}Ga_{0.25}$ $In_{0.5}$ P.

D. Conclusion

In this research, the optical properties of III-V quaternary compounds, AlGaInP used in high-brightness LEDs based on band structure, states density, fermi function, and carrier concentration have been evaluated. This research focuses on the computer-based simulation results for AlGaInP light-emitting diode modeling using mathematical equations. The analytical results have been discussed with detailed reports of the conditions. The research work approves the existing system from the literature background. A parabolic dispersion for AlGaInP has been calculated based on the physical parameters of the semiconductor materials. The required intensity and wavelengths need to be changed to mole fraction based on carrier concentration. To obtain the desired color emission of green and yellow LED depend the mole fraction of this compound on GaAs. $Al_{0.35}Ga_{0.15}$ $In_{0.5}$ P and $Al_{0.25}Ga_{0.25}$ $In_{0.5}$ P materials can be used as $(Al_xGa_{1-x})_{0.5}In_{0.5}$ P is closely lattice matched to the GaAs substrate, and it has a maximum direct bandgap energy of 2.321 eV (corresponding to 531 nm). According to the simulation results, the AlGaInP (yellow-green light-emitting diodes (LEDs)high brightness LEDs are well-suited for liquid crystal display applications.

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