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Design and simulation of single quantum well LED

Realized by :

Henka Ayman and Mesbahi Nidhal and Sakhri Med Hachani

Examination committee:

Dr. MEDJOURI Abdelkader	MCA	President
Dr. HIMA Abdelkader	MCB	Examiner
Pr. LAKHDAR Nacereddine	Pr	Director

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Abstract

Lighting is an essential component of economic activity in our modern society. It represents about 25% of the total electrical energy consumption globally. However, these lighting consume a lot of electricity produced mostly by polluting thermal power plants. Incandescent lamp has been the dominant component in lighting for over a hundred years despite an efficiency of only 17 lumens per watt .Today a new source of lighting is available that reduces the consumption of electricity and thus the production of greenhouse gases. Light-emitting diodes (LEDs), their energy efficiency, reliability and very long life can potentially overcome previous issues. Diverse types and structures have been previously studied in literature. In our work, single quantum well (SQW) LED based on InGaN material using Silvaco-Atlas software has been simulated and studied. The simulation results demonstrate that the device performance is considerably enhanced by the use SQW LED compared to that of standard LED. In addition, the effect of well-width on SQW design has been examined. Accordingly, the value of 47558 A/cm² is achieved in case of 2nm well-width, and it is better than 3nm and 2nm well-width. Clearly, the well-width of 2nm provides better performance compared to that of 3nm and 4nm.

Keywords: LED, single quantum well, IV characteristics, Silvaco-Atlas software.

Dedication

I thank God Almighty for giving me the strength, will and patience to complete my work. I would like to express my deepest and warmest gratitude to

Dr.LakhdarNacereddinefor supervising my memoir. I thank him very much for his hard work with us, and I thank all my professors who taught me throughout the university period. I also dedicate my work to

The source of my mother's tenderness and my father's source of love and safety.

And all of my friends and relatives wished me success, especially my mentor, Wael, for his moral support and motivation.

LIST OF SYMBOLS AND ABBREVIATIONS

LED	Light-Emitting Diode
OLED	Organic Light-Emitting Diode
AMOLED	Active Matrix OLED
EQE	External Quantum Efficiency
SCLC	Space-Charge-Limited Current
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
PTPB	polytetraphenylbenzidine
MO	metal–organic
FN	Fowler Nordheim
HTL	Hole Transporting Layer
ETL	Electron Transporting Layer
EML	Emissive Layer
SSL	solid-state lighting
FPDs	flat-panel displays
IESNA	Illuminating Engineering Society of North America
GaN	gallium-nitride
GaAsP	gallium-arsenic-phosphide
InGaN	indium-gallium-nitride
HID	high-intensity discharge

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General introduction

General introduction :

Lighting is an essential element of the economic activity in our modern society. However, these lighting consume a lot of electricity produced mostly by polluting thermal power plants. For this reason, a solution to reduce energy consumption is desirable from an economic and environmental point of view. Incandescent lamp has been the dominant component in lighting for over a hundred years despite an efficiency of only 17 lumens per watt. Today a new source of lighting is available that reduces the consumption of electricity and thus the production of greenhouse gases; we talk about SSL "solid state lighting", in other words about lighting by source in the solid state: it actually uses traditional semiconductor components of optoelectronics: high-intensity white light-emitting diodes (LEDs or light-emitting diodes), their energy efficiency, reliability and very long life. Previously used only as indicators on control panels (low-power LEDs), LEDs (high-intensity LEDs) are now finding applications in many areas such as road signs, car headlights or home lighting lamps, and this is thanks to technological advances in semiconductors, which now allow them to produce higher light levels than previous models. In this family, InGaN currently seems to be the most promising material for visible light emission. Interest in this material has increased since the advent of blue LEDs based on InGaN quantum wells, which paved the way for the production of white light sources with good lighting efficiency. On the other hand, as sources of electronic lighting, their mastery requires a number of skills ranging from optics to electronics, including Heat. The aim of our work is to study and model the single quantum well (SQW) LED structure using Silvaco-Atlas software. Therefore, standard and SQW LED designs are compared and results are shown in order to demonstrate the advantages of the SQW structure. For this reason, this memory is consists of three chapters, which are arranged as follows:

The first chapter is devoted to the presentation of light-emitting diodes. A Brief History, theory and principles of their operation are illustrated. In addition, different characteristics and their application in diverse domains are included. Chapter II describes various types of light-emitting diodes. We'll present the structure and operation principle of each type. In the third chapter, we will employ the program Silvaco-Atlas to the simulation and modeling of single quantum well LED structure. The different results are presented and discussed.

CHAPTER I:

Study of Light-emitting diodes (LEDs)

INTRODUCTION

Light-emitting diodes (LEDs) have become very popular and certainly have proven their usefulness in a wide variety of applications. These include applications requiring narrow-band color spectra [Tamulaitis, 2004] [1] [Harbers, 2007] [2] and indicative, decorative and signal lighting [Freyssinier, 2004] [3]. It cannot be denied that especially the high-power LED technology is developing very quickly and may be considered a promising alternative for general (public, industrial, private) lighting applications as well [Mottier, 2009] [4]. In this chapter, we start by the presentation of the history, theory, and structure of LED technology. Then, the advantages of LED will become even more evident by comparing it to current technologies and competitors in both industries. Therefore, the advantages and disadvantages of LED technology will be included.

1.1 History of LEDs :

The effect of light emission in response to the passing of an electrical current or a strong electric field is called electroluminescence and is the fundamental physical working principle of LEDs. Electroluminescence was discovered by H. J. Round of Marconi Labs in 1907 when he reported yellow electroluminescence from a piece of silicon carbide (SiC, also known as carborundum) [5]. These devices were Schottky diodes, rather than p-n diodes. Under strong forward bias conditions in these Schottky diodes, minority carriers are injected by tunneling from the metal and are able to recombine producing near-band gap light emission. The mechanism is similar in a p-n junction diode, yet the reported voltages required to turn on these Schottky devices ranged between 10 and 110V, much larger than those found in common LEDs [6].

Round's discovery was initially ignored and more than 20 years had to pass before the first report of an electroluminescent blue emitting device with accidental semiconductor p-n junctions. This work was published in 1928 by O.W. Lossew [7] who devoted the succeeding years to examining and describing this phenomenon in great detail. Following this work, G. Destriau came up with the term electroluminescence in 1936 when he discovered light emission from zinc sulfide [8]. The development of the transistor by J. Bardeen, W. Brattain and W. Shockley in 1947 provided a scientific step forward in semiconductor physics and revolutionized the field of electronics [9]. Shockley published "The theory of p-n junctions in semiconductors and p-n junction transistors" in 1949,

providing an explanation for the light emission effect in p-n junctions and a background for the study of p-n junction devices. New semiconductor growth techniques and consequent improvement of the quality of semiconductor films resulted in the first blue LED using SiC films with proper p-n junctions [10]. The drawback was the low electrical-to-optical power-conversion efficiency reported at this time of around 0.005% [11]. The reason for this low efficiency is that SiC has an indirect band gap so carriers cannot recombine without exchanging momentum with the crystal lattice. This radiative recombination process involving two carriers and a lattice phonon is very inefficient. III-V materials were postulated by H. Welker in 1953 [12] in the dawn of semiconductor science and technology. Previous studies were done with SiC and II-VI materials because many of these semiconductors occur in nature. III-V materials on the other hand, are manmade and require the careful growth of the material which had only recently become possible. The possibility of bulk growth of GaAs crystal structures allowed for example the demonstration of infrared LEDs and lasers in 1962 by M.I. Nathan et al. [13]. Some years later red LEDs were also demonstrated using GaAs crystals alloyed with GaP [14]. These early devices quickly showed promising electrical and optical properties although the external quantum efficiency of the alloy was limited to less than 0.03% at that time [15]. Nowadays these materials have been widely researched and the wide commercial availability of high quality GaAs bulk substrates allows for a relatively straightforward epitaxial growth of optoelectronic devices. Modern devices have reported external quantum efficiencies of 61% for red (650nm), 55% for orange-red (610nm) [16], while for the infrared case internal quantum efficiencies of at least 80% have been reported across the full 1.2 -1.6 μm band [17]. GaN is a wide band gap (3.41 eV) III-V semiconductor capable of emitting light in violet and blue colours by direct band gap emission. This material has been known since the first half of the 20th century when a publication by R. Juza and H. Hahn [18] (1938) described how to prepare GaN powder by reacting ammonia with liquid gallium metal at high temperatures. These studies formed the basis for the work of H. P. Maruska and J. J. Tietjen on the growth of GaN single-crystal films three decades later (in 1969) using sapphire as a substrate [19]. During the next decade of the 1970's several groups took an interest in the development of GaN crystals with the strong belief that these crystals could yield the first efficient blue LED. The main problem faced at this time was how to achieve the required p-doping of the GaN to form a p-n

junction. These originally reported GaN thin films were all n-type without intentional doping. Zinc was the first element used as an acceptor dopant for GaN but even under heavy Zn concentrations GaN only proved to be insulating [6]. Although not a LED device, these early efforts resulted in the first metal-insulator-semiconductor (MIS) diode demonstrated in 1971 by Pankove et al. [20]. This device had an emission wavelength of 475nm which makes it the first GaN-based current-injected device capable of emitting light. The unavailability of p-type GaN led to the momentary abandonment of the research in GaN as a material for blue LEDs until 1989 when I. Akasaki et al. demonstrated the first true p-type doping and p-type conductivity in GaN [21]. They used Mg following previous works from H. P. Maruska, although to achieve p-conductivity in this case Mg dopants were activated after the growth of the material. The first way of activating these dopants was using electron-beam irradiation [21] and later it was demonstrated by Nakamura et al. [22] that the activation could be done by post-growth thermal annealing. Nowadays, thermal annealing is the standard procedure to activate p-dopants and achieve p-type GaN thin films. Once the possibility of creating a p-n homo junction with GaN had become a reality, the interest in the material started to grow again and in 1993 the first viable blue [23] and violet [24] InGaN double heterostructure LEDs were demonstrated by Nakamura et al. reporting external quantum efficiencies of 0.22% and 0.15%, respectively. Their work also led to the development of the first green GaN LEDs a couple of years later [25]. I. Akasaki, H. Amano and S. Nakamura were awarded the Nobel prize in Physics in 2014 “for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources” [26].

1.2 Luminous Intensity over the year:

The following graph shows the improvement of luminous intensity of LEDs over the years.

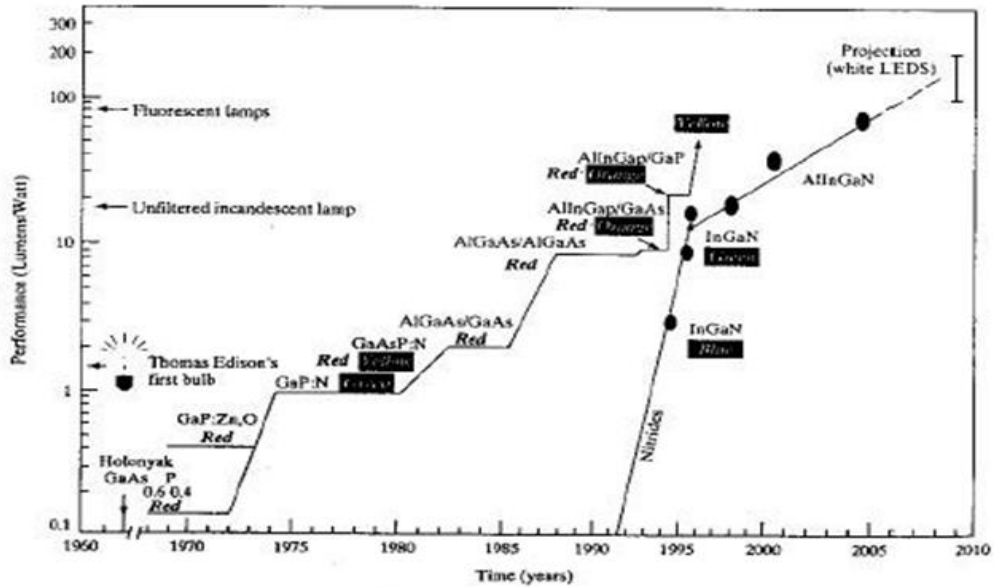
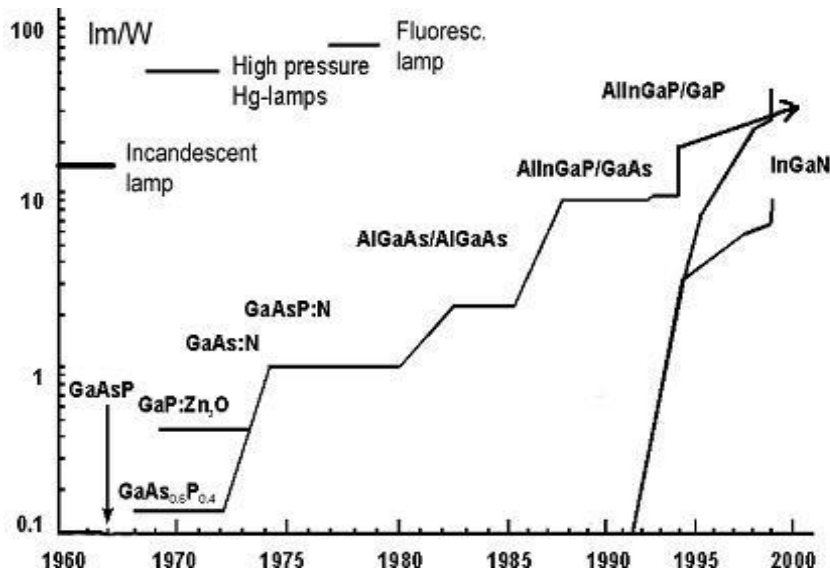


Figure 1 :Improvement of luminous intensity of LEDs over time.[Modified from M.G.Craford. IEEE Circuits and Devices. p. 24/sept/1992].[27].

The following graph shows how the efficacy of III-V compound LEDs could be increased by introducing new compositions. The first visible light emitting diodes were fabricated using a GaAsP alloy.[27].



1.3 Theory of LEDs :

At the abrupt interface of p-type and n-type material, with donor concentration N_D and acceptor concentration N_A , we can consider all the dopants ionised such that the free electron concentration is given by $n = N_D$ and the free hole concentration is given by $p = N_A$. At the unbiased p-n junction, free electrons supplied by the donor atoms diffuse over to the p-type region where they recombine with a hole, a corresponding process occurs with holes diffusing into the n-type region. With the free carriers near the junction depleted the ionised donors and acceptors produce spatially separated electrical charges. The separated charges result in an electric potential known as the diffusion

Voltage (V_D) which stops further diffusion and has a value which is given by [28]: $V_D = \frac{KT}{e} \ln \frac{N_A N_D}{n_i^2}$

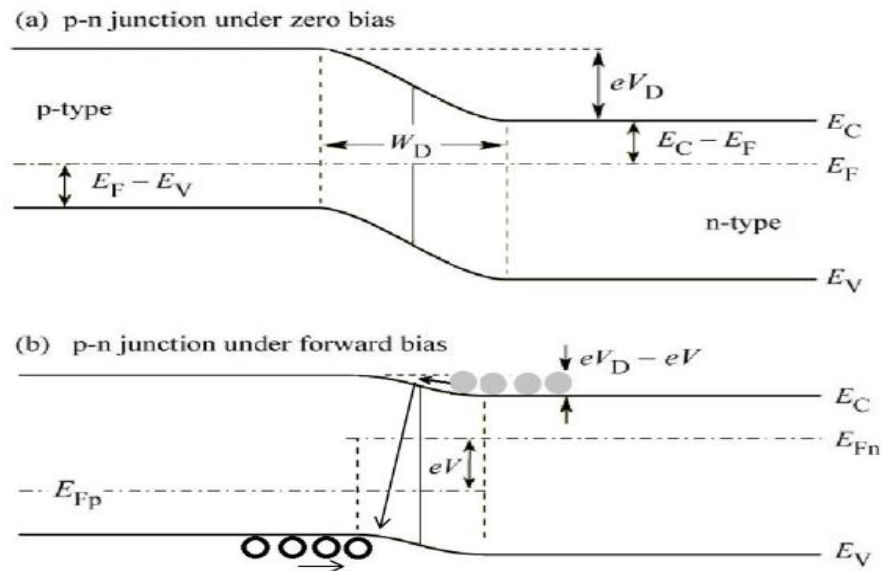


Figure 2.1: (a) An unbiased p-n junction showing the diffusion voltage (V_D) and depletion region width (W_D). (b) The same p-n junction under a forward bias (V) electrons are light grey and holes are hollow circles [29].

Where N_A and N_D are the acceptor and donor concentrations, respectively, k is the Boltzmann constant, T is the temperature, e is the charge of an electron and n_i is the intrinsic carrier concentration. These properties are illustrated in Figure 2.10. Between the two regions there are no longer free carriers, this region is known as the depletion region.

The width of this region (W_D) is given by [29]: $W_D = \sqrt{\frac{2\epsilon}{e} (V_D - V) \left(\frac{1}{N_A} + \frac{1}{N_D} \right)}$

Where ϵ is the permittivity of the semiconductor and V is the bias voltage. This can be seen in Figure 2.1.

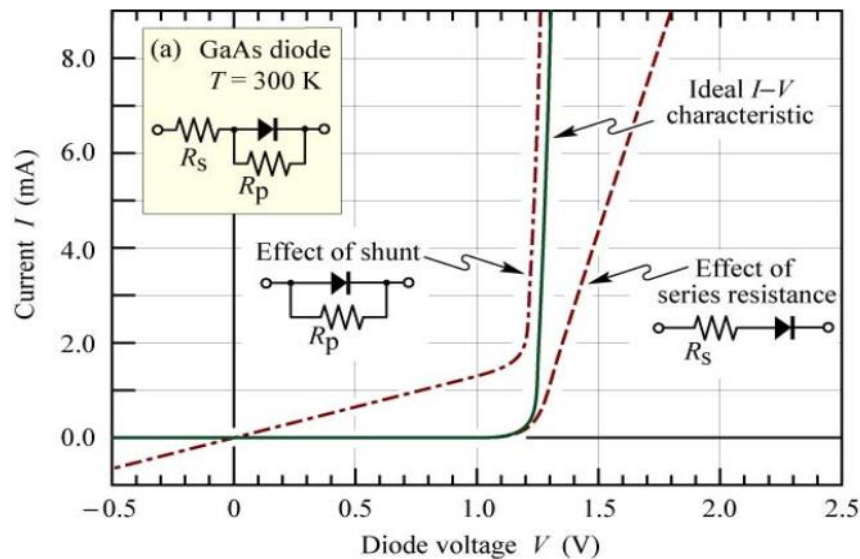


Figure 2.2: The effect of series and parallel (shunt) resistances in the current voltage relation of an LED[29]

Under forward bias the depletion region is injected with electrons and holes, electrons in the n-type and holes in the p-type. They diffuse through to the depletion region before eventually recombining once spatially close enough and producing a photon. As the bias voltage is increased the current flow increases. The diode equation was first developed by Shockley and is thus known as the Shockley equation[30]: $I = I_S(e^{e(V-V_D)/KT} - 1)$

Where I_S is the reverse bias saturation current.

In real diodes there are several deviations from an ideal diode equation, these are shown in equation. An ideality factor n_{ideal} is required. In a perfect diode all current would be due to diffusion, this would give an ideality factor of 1, the presence of recombination and generation of carriers results in a value of $n_{ideal} = 1.1-1.7$ being a combination of diffusion and carrier generation and recombination. The ideal diode equation also doesn't take into account any un-wanted resistances, these can either be series or parallel resistances. Series resistances are caused by excessive contact resistance or the neutral regions of the device. Parallel resistances occur when a current can bypass the p-n

junction either through defects such as threading dislocations or surface imperfections. The effects of these resistances on the IV characteristics of an LED are shown in Figure 2.2,

$$I - \frac{(V-IR_S)}{R_P} = I_S \left(e^{e(V-IR_S)/n_{ideal} KT} \right)$$

Therecombination can be classified intothe following two kinds

- A)-Direct recombination
- B)-Indirect recombination

A)-DirectRecombination:

In direct band gap materials, the minimum energy of the conduction band lies directlyabove the maximum energy of the valence band in momentum space energy (Figure 2.3 shows the E-k plot [31] of a direct band gap material). In this material, free electrons at the bottom of the conduction band can recombine directly with free holes at the top of the valence band, as the momentum of the two particles is the same. This transition from conduction band to valence band involves photon emission (takes care of the principle of energy conservation). This is known as direct recombination. Direct recombination occurs spontaneously. GaAs is an example of a direct band gap material.

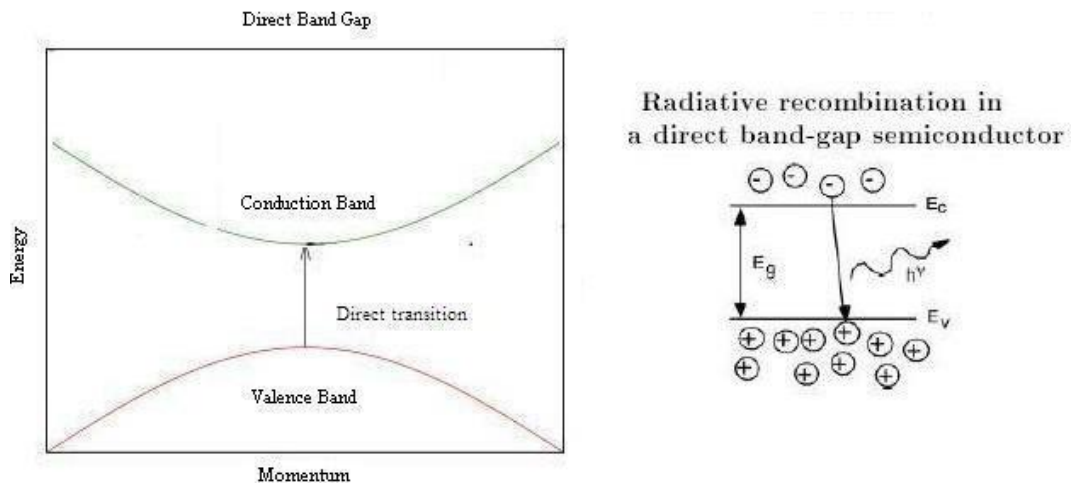


Figure 2.3: Direct Bandgap and Direct Recombination

B)-IndirectRecombination:

In the indirect band gap materials, the minimum energy in the conduction band isshifted by ak-vector relative to the valence band. The k-vector difference represents a

difference in momentum. Due to this difference in momentum, the probability of direct electron-hole recombination is less. In these materials, additional dopants (impurities) are added which form very shallow donor states. These donor states capture the free electrons locally; provides the necessary momentum shift for recombination. These donor states serve as the recombination centers. This is called Indirect (non-radiative) Recombination. Figure 2.4 shows the E-k plot of an indirect band gap material and an example of how Nitrogen serves as a recombination center in GaAsP. In this case it creates a donor state, when SiC is doped with Al, its recombination takes place through an acceptor level. The indirect recombination should satisfy both conservation energy, and momentum. Thus besides a photon emission, phonon emission or absorption has to take place.

GaP is an example of an indirect band gap material.

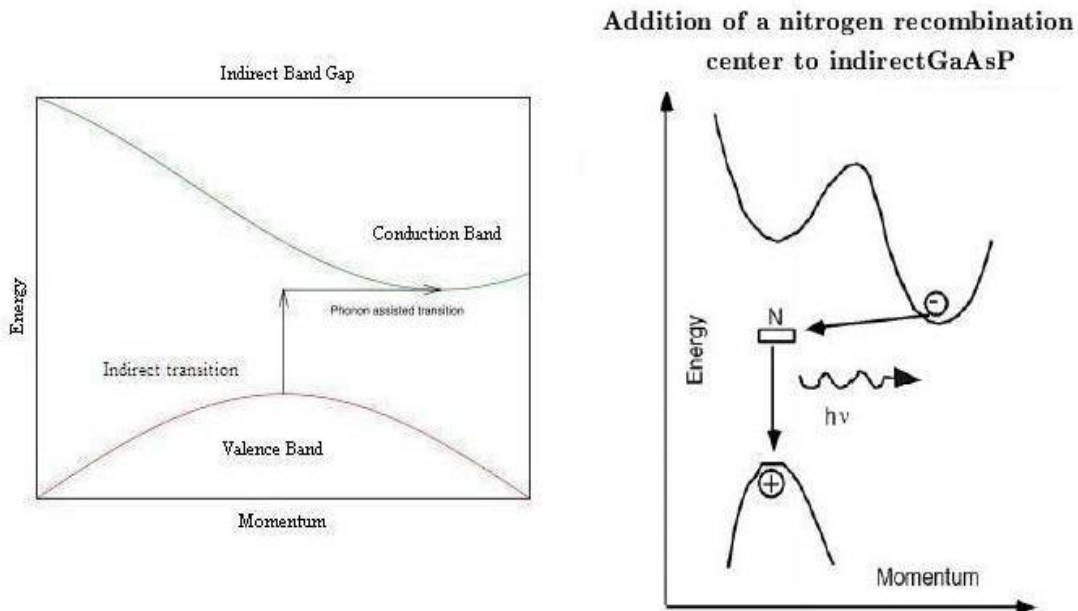


Figure 2.4: Indirect Band gap and Non Radiative recombination

The wavelength of the light emitted, and hence the color, depends on the band gap energy of the materials forming the p-n junction. The emitted photon energy is approximately equal to the band gap energy of the semiconductor. The following equation relates the wavelength and the energy band gap.

$$h\nu = \frac{hc}{\lambda} = E_g$$

$$\lambda = \frac{hc}{E_g}$$

- Where h is Planck's constant, c is the speed of the light and E_g is the energy band gap. Thus, a semiconductor with a 2eV band gap emits light at about 620nm, in the red. A 3eV band gap material would emit at 414nm, in the violet. [32] shows a list of semiconductor materials and the corresponding colors.

1.4 LED Efficiency :

The efficiency of a light emitting diode can be separated into three groups. First the extraction efficiency (n_{ext}) describes the fraction of photons generated that actually get out of the device. This can be referred to as the packaging challenge. Once photons are generated, losses can occur due to total internal reflection, internal reabsorption, and contact blocking. Another issue in extraction efficiency is desired radiation pattern.

Second, the internal quantum efficiency (n_i) describes the fraction of electrical current that contributes to excited carriers that recombine before reaching the contacts. Materials are desired that have short radiative recombination lifetimes and the diodes must be long enough to sustain these lifetimes and encourage recombination. Creative structures such as quantum wells aid in improving this efficiency by providing an energy trap where carriers do not have energy to escape once they are within the wells. Since they are trapped, they will surely recombine. Efforts should be made to reduce contact resistance and bulk resistance so most or all of the voltage drop occurs at the PN junction. This insures minimal electrical power loss. Device engineering and design are crucial in improving this efficiency.

Finally, radiative efficiency (η_{rad}) describes the fraction of excited carriers that recombine radiatively, as opposed to non-radiatively. This efficiency relies on material selection and quality of material. Foremost, an LED requires a direct band gap semiconductor to have any significant radiative recombination at all. However even direct band gap semiconductors can have deep level traps which lead to non-radiative recombination. Care must be taken to grow materials of very high quality with few defects to ensure higher radiative efficiency. Smaller radiative recombination lifetimes and larger non-radiative recombination lifetimes are desired. Furthermore, surface traps and interface

traps between the p and n semiconductors can also lead to increased non-radiative recombination's.

The external quantum efficiency (EQE) of the entire light emitting diode is merely a product of the three different efficiencies described here. This EQE relates the final power output of the photons to the input electrical power.

1.5 LED Structure:

The LED structure plays a crucial role in emitting light from the LED surface. The LEDs are structured to ensure most of the recombination's takes place on the surface by the following two ways.

- By increasing the doping concentration of the substrate, so that additional free minority charge carriers electrons move to the top, recombine and emit light at the surface.
- By increasing the diffusion length $L = \sqrt{D\tau}$, where D is the diffusion coefficient and τ is the carrier life time. But when increased beyond a critical length there is a chance of reabsorption of the photons into the device.

The LED has to be structured so that the photons generated from the device are emitted without being reabsorbed. One solution is to make the p layer on the top thin, enough to create a depletion layer. Following picture shows the layered structure. There are different ways to structure the dome for efficient emitting [33].

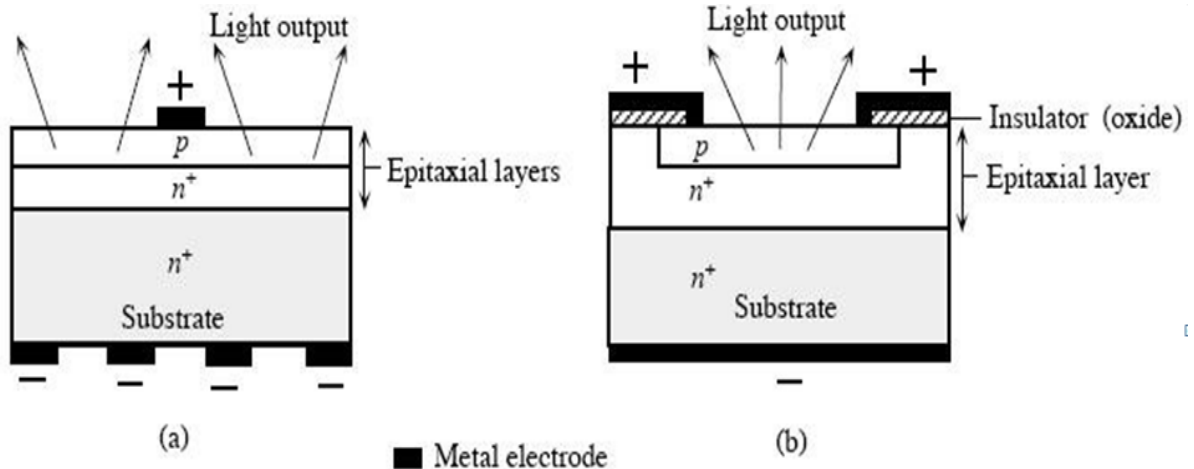


Figure 3: LED structure [33].

A schematic illustration of typical planar surface emitting LED devices.

(a) p-layer grown epitaxial on an n^+ substrate.

(b) First n^+ is epitaxial grown and then p region is formed by dopant diffusion into the epitaxial layer.

LEDs are usually built on an n-type substrate, with an electrode attached to the p-type layer deposited on its surface. P-type substrates, while less common, occur as well. Many commercial LEDs, especially GaN/InGaN, also use sapphire substrate [33].

1.6 Applications: LEDs have a lot of applications. Following are a few examples.

- Devices, medical applications, clothing, toys
- Remote Controls (TVs, VCRs)
- Lighting
- Indicators and signs
- Optoisolators and optocouplers
- Swimming pool lighting

1.7 Advantages of LEDs :

- LEDs produce more light per watt than incandescent bulbs; this is useful in battery-powered or energy-saving devices.
- LEDs can emit light of an intended color without the use of color filters that traditional lighting methods require. This is more efficient and can lower initial costs.
- The solid package of the LED can be designed to focus its light. Incandescent and fluorescent sources often require an external reflector to collect light and direct it in a suitable manner.
- When used in applications where dimming is required, LEDs do not change their color tint as the current passing through them is lowered, unlike incandescent lamps, which turn yellow.
- LEDs are ideal for use in applications that are subject to frequent on-off cycling, unlike fluorescent lamps that burn out more quickly when cycled frequently. Or High Intensity Discharge (HID) lamps that require long time before restarting.

- LEDs, being solid state components, are difficult to damage with external shock. Fluorescent and incandescent bulbs are easily broken if dropped on the ground.
- LEDs can have a relatively long useful life. A Philips LUXEON k2 LED has a life time of about 50,000 hours, whereas Fluorescent tubes typically are rated at about 30,000 hours, and incandescent light bulbs at 1,000–2,000 hours.
- LEDs mostly fail by dimming over time, rather than the abrupt burn-out of incandescent bulbs.
- LEDs light up very quickly. A typical red indicator LED will achieve full brightness in microseconds; Philips Lumileds technical datasheet DS23 for the Luxeon Star states "less than 100ns." LEDs used in communications devices can have even faster response times.
- LEDs can be very small and are easily populated onto printed circuit boards.
- LEDs do not contain mercury, unlike compact fluorescent lamps.

1.8 Disadvantages :

- LEDs are currently more expensive, price per lumen, on an initial capital cost basis, than more conventional lighting technologies. The additional expense partially stems from the relatively low lumen output and the drive circuitry and power supplies needed. However, when considering the total cost of ownership (including energy and maintenance costs), LEDs far surpass incandescent or halogen sources and begin to threaten the future existence of compact fluorescent lamps.
- LED performance largely depends on the ambient temperature of the operating environment. Over-driving the LED in high ambient temperatures may result in overheating of the LED package, eventually leading to device failure. Adequate heat-sinking is required to maintain long life.
- LEDs must be supplied with the correct current. This can involve series resistors or current regulated power supplies.
- LEDs do not approximate a "point source" of light, so they cannot be used in applications needing a highly collimated beam. LEDs are not capable of

providing divergence below a few degrees. This is contrasted with commercial ruby lasers with divergences of 0.2 degrees or less. However this can be corrected by using lenses and other optical devices.

- There is increasing concern that blue LEDs and white LEDs are now capable of exceeding safe limits of the so-called blue-light hazard as defined in the eye safety specifications for example ANSI/IESNA RP-27.1-05: Recommended Practice for Photo biological Safety for Lamp and Lamp Systems.

Conclusion

The most important difference between an LED and a diode is that the LED emits light while the diode allows the current to flow in only one direction and opposes the flow in the opposite direction. (LED) is a kind of diode made of germanium arsenic or germanium phosphide.

Also we know that the light of different colors is emitted by the LED. In this nature, we can differentiate lamps. Due to the semiconductor materials used during the formation of the diode, the device emits different colors of light. Among the advantages of LED over the usual means of illumination are brighter, shorter response time, lighter weight, more rigidity and a wider temperature range.

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ChapterII:

Different type of LED structures (designs)

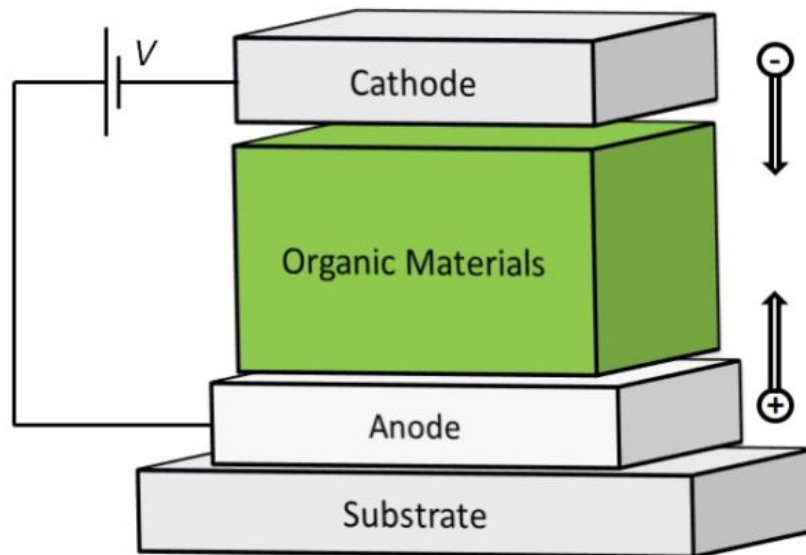
INTERODICATION

In this chapter, diverse type of LED structures will be presented in detail. In each of these structures, we will demonstrate a design and working principle. In addition, applications and difference between them will be presented.

2.1organic LED :

2.1.1 Design of organic LED Architecture:

In their simplest form, OLEDs are electroluminescent devices consisting of multiple organic layers sandwiched between two electrodes (an anode and a cathode) [34] . Figure 4 shows a simplified illustration of a single layer OLED. In this particular configuration, holes and electrons are injected and transported through the organic material under a forward bias voltage V , with the positive terminal connected to the anode and the negative terminal connected to the cathode. These charges work their way through the organic materials, towards the center of the device under the influence of the applied electric field and recombine in the form of electron-hole pairs called excitons. Light is emitted when these excited states decay and release their energy through the emission of a photon, which exits the device through either a semi-transparent anode or cathode.



2.1.2 Working principle of OLEDs

During operation, a voltage is applied across the OLED such that the anode is positive with respect to the cathode. A current of electrons flows through the device from cathode to anode, as electrons are injected into the LUMO of the ETL at the cathode and withdrawn from the HOMO of the HTL at the anode. This latter process may also be described as the injection of holes. Then holes and electrons drift through the organic layers toward each other under the influence of the external electric field. Some of these carriers recombine to form excitons. This happens in the EML and usually closer to the EML/ETL interface, because in organic semiconductors holes are generally more mobile than electrons. Some exciton decay routes are radiative, leading to light emission. The photon energy E_{photon} depends on the band gap E_g of the emitter material, in this case the difference in energy between the HOMO and LUMO. Therefore, basically, light emission from OLEDs is governed by three major electronic processes: charge injection, transport, and recombination. The resistivity of a typical organic material is in the range of $10^{15} - 10^{20} \Omega\text{cm}$ at low electric fields ($<10^4 \text{ V/cm}$), which is too high to be considered as a good electric conductor, even semiconductor. This is the reason that the total thickness of the organic layers in the OLEDs usually is $\sim 100 \text{ nm}$. This extremely low conductivity also implies that organic semiconductors intrinsically have virtually no free charge carriers, so charge carrier injection is one major step in charge transport in OLEDs. Inefficient injection or extraction of charge will hamper the device performance. In general, there are three major theoretical approaches involved to describe the charge injection mechanism:

- 1) Field-assisted thermionic injection in which the carriers from the electrodes are thermally excited to overcome the potential barrier resulting from the superposition of the image charge potential and external field [35].

$$J = J_{\text{inj}} - J_{\text{rec}} = A^* T^2 e^{-\frac{\phi_B}{kT}} e^{f^{1/2}} - n_0 q S^{(F)}$$

Where $A^* = \frac{16\pi\epsilon\epsilon_0 K^2 N_0}{q^2}$ is the effective Richardson constant, $f = \frac{qfr_c}{KT}$ is the reduced electric field and $S = \frac{J_{\text{rec}}}{n_0 q}$ is the surface recombination velocity. At high temperatures or low injection barrier heights, thermionic emission predicts the injection of a charge carrier from a metal contact into a semiconductor if the thermal energy of the carrier is greater than the Schottky barrier height.

- 2) The Fowler Nordheim (FN) tunneling injection model, in which the carriers tunnel through the potential barrier of the metal–organic (MO) contact under a high electric field [36-38]:

$$J = AF^2 e^{-\frac{8\pi\sqrt{2m^*}\phi_B^{1.5}}{3\hbar eF}}$$

where m^* is the effective charge carrier mass, F is the applied electric field, and $A = \frac{q^3}{8\pi\hbar\phi_B}$ is a rate coefficient that contains a tunneling prefactor and the rate of current back-flow. At high electric fields or high injection barrier heights, the FN model describes tunneling currents through a triangular barrier into a delocalized conduction band. 3) The thermo activated hopping injection model, which is attributed to the hopping of carriers from the metal Fermi level into the localized states of the organic semiconductor [39-44]. The results from the model were found to successfully describe the temperature and injecting contact-dependent current–voltage characteristics in a polytetraphenylbenzidine (PTPB).

In all of these approaches, the injection process is dominated by the charge injection barriers at the interfaces between the active layers and the metal electrodes. Injection barriers can be difficult to estimate from the work function of the metal electrode and the HOMO (or LUMO) of the organic layer. Actual injection barrier heights can deviate quite strongly from the expected values. Those deviations are attributed to chemical reactions between the metal and semiconductor leading to interface dipoles [45-46] band bending [47-48], or Fermi level pinning [49]. As a rule of thumb, the currents in organic devices with injection barriers greater than 0.25–0.3 eV [50] at zero field are found to be ‘injection limited’, i.e., the maximum current is determined by the injection process of the charge carriers into the device, as opposed to ‘bulk limited’ (or space-charge limited) devices (see below).

The charge carrier mobilities in organic semiconductors are typically low and Ohm’s law is followed at a very low V . If the injection barriers are small, and the electrode can supply more carriers per unit time than can be transported through the bulk, the current is limited by the latter and can be described using the theory of space-charge-limited currents (SCLC) [50,51–53]. Such organic/metal contacts are said to be Ohmic contacts

$$J_{\text{SCL}} = \frac{9 \epsilon \epsilon_0 \mu V^2}{8 L^3}$$

Here, ϵ_0 is the permittivity of free space, ϵ is the relative dielectric constant, μ is the microscopic mobility of the carriers, L is the thickness of the organic film, and V is the voltage.

2.1.3 Applications of OLEDs

OLED technology is realized in commercial applications such as flat-panel displays (FPDs) and solid-state lighting (SSL).

- 1) Flat-panel displays: I. Small screens: OLEDs used as small screens in mobile phones, portable digital media players, car radios, digital cameras, and others. Such portable applications favor the high light output of OLEDs for readability in sunlight and their low power drain. OLEDs are also used in many Motorola and Samsung cell phones, as well as some HTC, LG and Sony Ericsson models [54]. Nokia has also recently introduced some OLED products including the N85 and the N86 8MP, both of which feature an AMOLED display. OLED technology can also be found in digital media players such as the Creative ZEN V, the iriver clix, the Zune HD, and the Sony Walkman X Series. II. TVs

OLED-TVs are commercially available now. DuPont stated in a press release in May 2010 that they can produce a 50" OLED TV in two minutes with a new printing technology [54].

- 2) Solid-state lighting: Applications in flexible signs and lighting are also being developed [55]. Philips Lighting has made OLED lighting samples under the brand name 'Lumiblade,' which are available for sale online [56] and Siemens Osram offers the Orbeus white OLED panels for sale.

2.2 Homojunction LEDs:

The homojunction LED is the simplest LED structure, consisting of a p-n junction realized with a single material. In such a structure, the carrier distribution depends on the diffusion constant of the carriers. Under forward bias, electrons will diffuse from the n-side to the p-side, while holes will diffuse from the p-side to the n-side and eventually will recombine with majority carriers. The mean distance that a minority carrier diffuses before recombination is the diffusion length, which is equal to $L_n = \sqrt{D_n \tau_n}$ and $L_p = \sqrt{D_p \tau_p}$ for

electrons and holes, respectively. We can see that the carrier distribution along the junction is proportional to the diffusion constant, and thus to the carrier mobility, and to their lifetime.

In typical semiconductors, the diffusion length is in the order of a several micrometers. For example, the diffusion length of electrons in p-type GaAs is equal to $L_n \approx 15 \mu\text{m}$ and thus the minority carriers are distributed over a region several micrometers thick [57]. Figure 5 shows the carrier distribution in a p-n homojunction under zero bias and under forward bias, respectively. Note that minority carriers are distributed over a quite large distance under forward bias condition. Thus, recombination occurs over a large region, with a strongly changing of minority carrier concentration. The large recombination region in homojunctions is not beneficial for efficient recombination. This is due to the fact that the radiative recombination rate $R = Bnp$ is proportional both to electron and hole concentration and, as we have seen above, these concentrations are quite low in this structure. For this reason, p-n homojunction structure is not usually employed for the realization of LEDs.

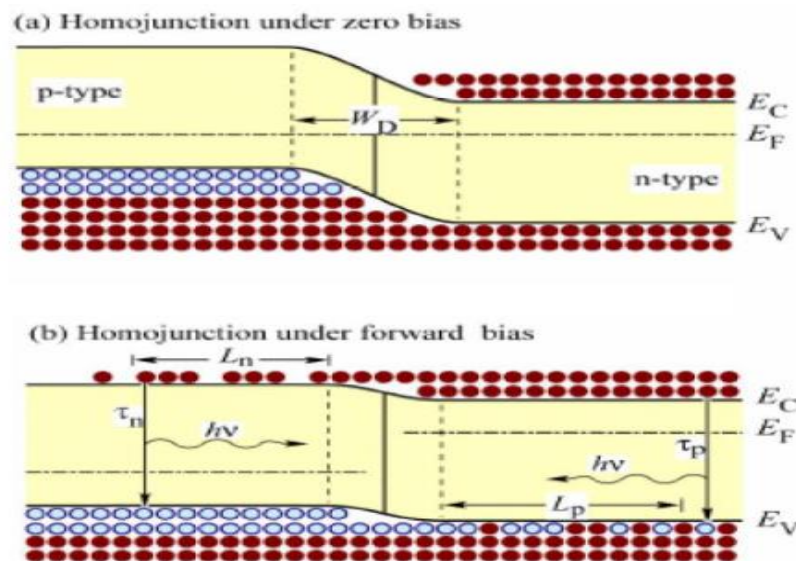


Figure 5: Carrier distribution in a p-n homojunction under (a) zero bias and (b) forward bias

2.3 Heterojunction LEDs :

All high-intensity light-emitting diodes do not use the homojunction design but rather employ heterojunction structures, which have clear advantages over homojunctions devices. Heterojunction devices employ two types of semiconductors, with different

energy gap and other physical properties, such as the dielectric permittivity. As in homojunction LEDs, also in heterojunction LEDs materials with different conductivity (i.e. both n-type and p-type doped materials) are usually employed, even if interesting results can be obtained also employing materials with different energy gap and the same type of doping. When a p-n heterojunction is formed, electrons diffuse from the n-side to the p-side and holes diffuse from the p-side to the n-side, as in a p-n homojunction. However, because of the different energy gap and electronic affinity between different materials, the carrier diffusion creates discontinuities both in the conduction band (ΔE_c) and in the valence band (ΔE_v), as shown in Figure 6 for a generic heterojunction between two different semiconductors. In particular, from the Anderson's theory results:

$$\Delta E_c = q(\chi_1 - \chi_2) \text{ And } \Delta E_v = \Delta E_g - \Delta E_c$$

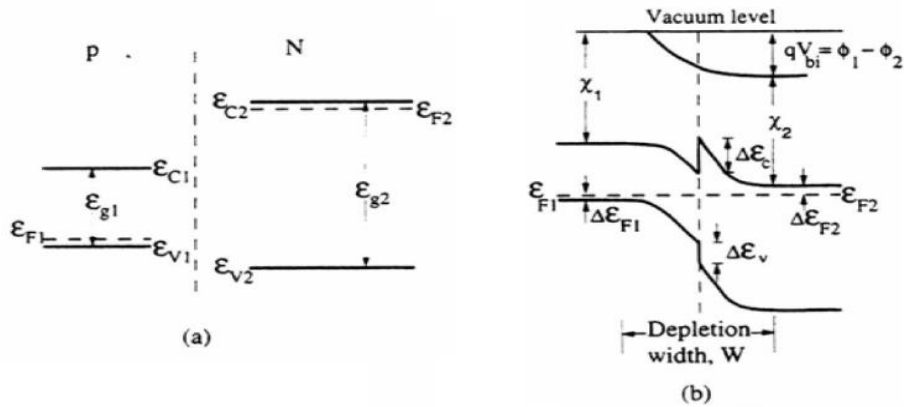


Figure 6: Band diagram (a) before and (b) after the formation of a heterojunction between two semiconductors with different energy gap. The band diagram on the right-hand is referred to the equilibrium condition under zero bias.

In order to understand how heterostructures can influence the carrier distribution in the proximity of junction, we consider the heterojunction of Figure 5 when a forward bias is applied. An increase in the forward voltage reduces the electron barrier: the results of applied bias is shown in Figure 7: as it can be noticed, the discontinuity ΔE_c in the conduction band does not slow the electron flow. On the other hand, even if also the barrier to hole flow is reduced, the discontinuity ΔE_v in the valence band does not change with

increasing the forward voltage, thus strongly slowing the hole flow towards the n-side. As a result, a hole confinement was obtained in such a structure, thus increasing its concentration in proximity of the junction. Therefore, the radiative recombination probability results increased with respect to the homojunction structure. However, from Figure 7 it is clear that it is not possible to obtain simultaneous confinement of both electron and holes in the same region. For this reason, even if a single heterojunction results in an improved radiative efficiency, it is not the best solution to obtain LEDs with high efficiencies.

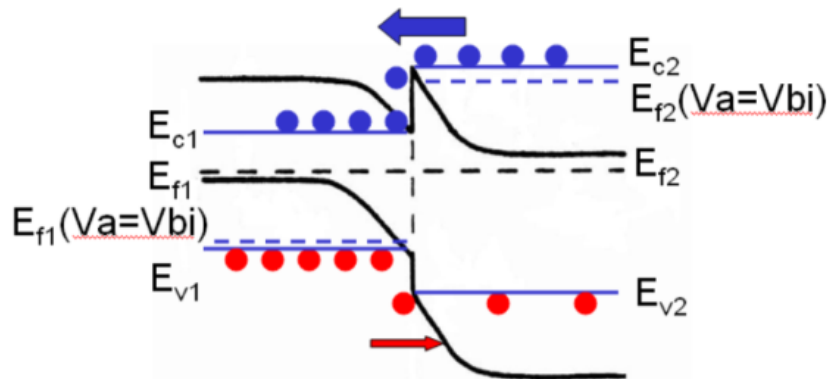


Figure 7: Carrier distribution in a p-n heterojunction under forward bias condition.

A better solution that permits to obtain very high internal quantum efficiency is the double heterostructure (DH). It consists of two barriers, which are obtained by interposing a small band-gap semiconductor, usually indicated as the active region, between two semiconductor layers having a greater energy gap with respect to the active region. The effect of heterojunction on the carrier distribution is shown in Figure 8: as it can be noticed, carriers injected in the active region of the double heterostructure are confined to this zone by means of the barriers. As a result, the thickness of the region in which carriers recombine is given by the thickness of the active region, than rather the diffusion length. If the active region thickness is appropriately chosen, the radiative recombination rate can be strongly increased with respect to the homojunction structure, because the carriers in the active region of a double heterostructure have a much higher concentration than carriers in

homojunctions. For example, the diffusion length of carriers may range from 1 to 20 μm . On the other hand, the active region of a double heterostructure may range from 0.01 to 1 μm .

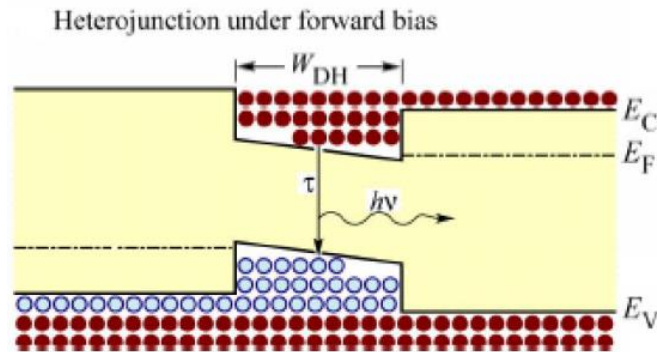


Figure 8: Carrier distribution in a double heterostructure (DH) under forward bias.

Double heterostructures can also be used to confine light to waveguide regions: this can be obtained thanks to the difference between the refractive index of active region and barrier layers. In particular, optical confinement is used for the realization of edge-emitting LEDs [57]. Moreover, due to the smaller energy gap of the active region with respect to the barrier layers, emitted photons from the active region will not be reabsorbed by barriers, thus further increasing the optical efficiency of devices. However, heterostructures are characterized by also some drawbacks, which can limit the optical efficiency of devices, including:

- increased device resistance caused by the heterointerfaces
- carrier loss in double heterostructures
- carrier overflow in double heterostructures
- lattice strain due to the lattice mismatch between different semiconductor materials.

In the following, we will briefly analyze each of these drawbacks

2.4 Heterostructures LEDs :

One approach to achieve a higher concentration of carriers is to use a heterostructure [58]. Unlike the p-n homojunction the heterostructure uses two different semiconductor materials with different band gaps. One small bandgap material is used as the active region and one large bandgap material is used as the barriers. The small band gap material is undoped and sandwiched between two pieces of doped large bandgap materials. A relevant example is

InGaN as the active region with GaN barriers on the sides. The description above is actually called a double heterostructure because there are two interfaces between the small and the large bandgap materials. The point of a double heterostructure is that it works as a quantum well. Carriers that are injected into the active region (small band gap material) will be confined. They are forced into the energy bands of the active region rather than diffusing far into the opposite sides. There will thus be a large amount of carriers in the valence and conduction band of the active region which benefits the radiative recombination rate. Electrons and holes will thus recombine in the active region. The width of the active region is usually in the order of a few nanometers which, compared to the diffusion length of several micrometers, is very small. The issue of uneven distribution of carriers will thus be reduced by the use of a double heterostructure.

Figure 9 shows both a homojunction and a double heterostructure. In the heterostructure carriers are confined in the quantum well and will recombine in the small band gap material. The small band gap material is often called “active region” because it is the place where recombination occurs. The photons emitted from the active region will have a wavelength determined by the active region band gap. The bandgap of the substrate and barrier material will thus be larger than the photon energy which reduces the probability of absorption.

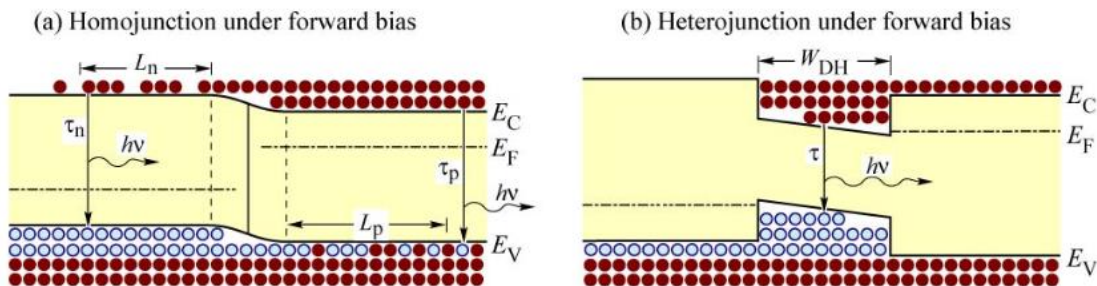


Figure 9: a) Homojunction and b) Heterostructure. [59]

Creating a double heterostructure requires two semiconductor materials with desired band gaps and matching lattice constants. This is usually the most challenging part where lattice mismatch and dislocations at the interfaces become an issue. This is a significant challenge when fabricating green or other long wavelength LEDs. Dislocations at the interfaces will usually result in poor efficiency and promote non-radiative recombination.

Conclusion

After this study, we conclude that the p-n homojunction structure is not usually used to realize LEDs due to the low concentration of electrons in this architecture, also heterojunction is not the best solution for obtaining high efficiency LEDs. However, heterostructures is one of the methods to achieve higher concentration for obtain high-efficiency LED lights, and the radiative composition is higher than the homojunction and heterojunction structure.

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Chapter III:

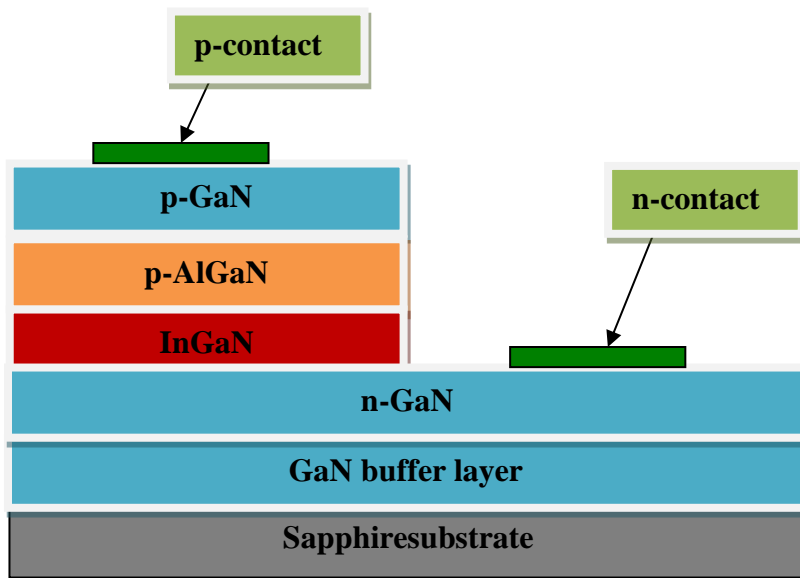
Modeling and simulation

INTERODICATION

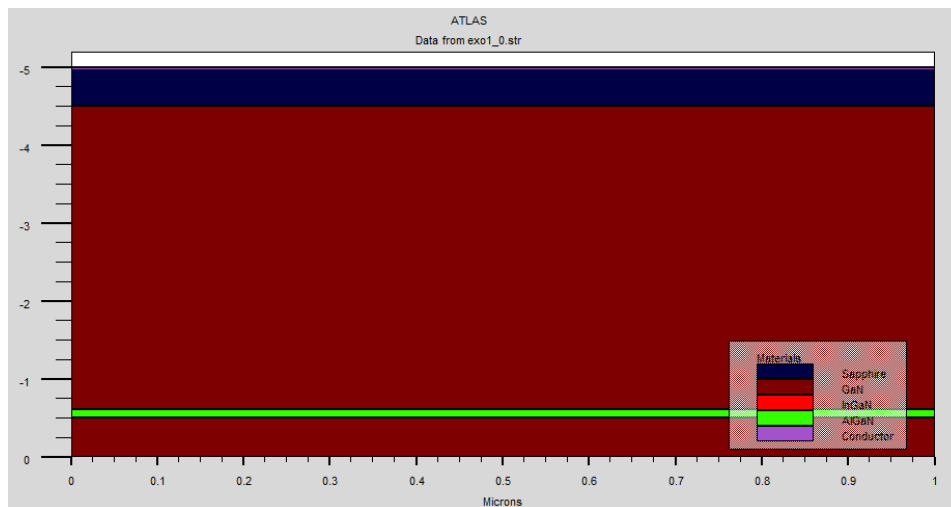
In order to simulate the electrical and optical characteristics of our blue light emitting diode based on quantum well InGaN. In this chapter, we will use the software "Silvaco-Atlas" by explaining the steps followed to simulate our proposed structure. The single quantum well LED will compared with that of conventional structure and the results will be presented. Therefore, the influence of well width on I-V characteristics is also illustrated.

3.1 Description of the simulated LED structure:

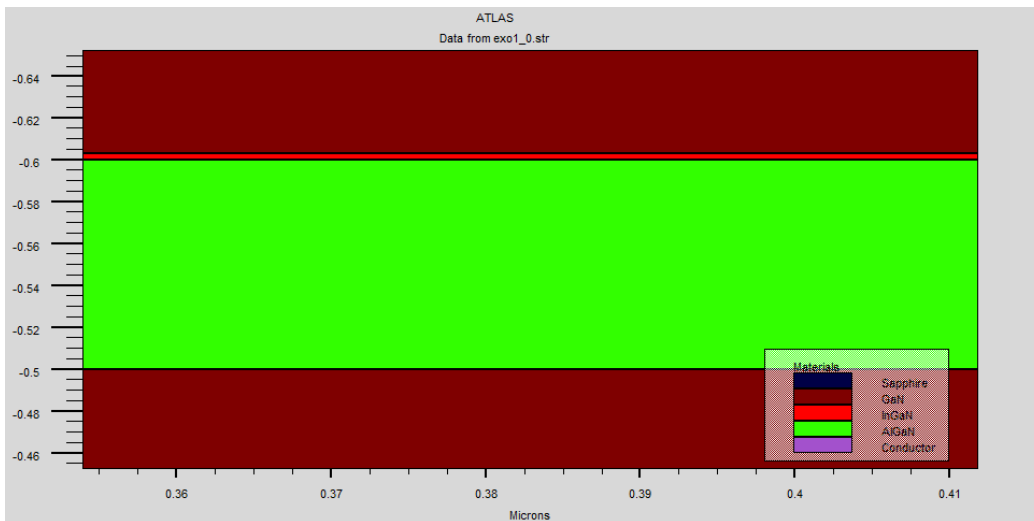
A bibliographic study on different structures of light-emitting diodes allowed us to fix our choice on the blue LED with single quantum well based on indium gallium nitride InGaN. The objective of this work is to make a design by simulation under ATHENA. To define the technological parameters necessary for the simulation, such as layer thicknesses, doping as well as certain electrical parameters, we based ourselves on values found in the literature, concerning the study of different structures of light-emitting diodes. Figure 10 shows the studied structure of single quantum well LED. This latter consists of five regions deposited on sapphire substrate (fig.1a). Starting with undoped GaN layer of $0.3\mu\text{m}$ thickness. Followed by a layer of n-GaN with $4\mu\text{m}$. A thin region of undoped InGaN which represents a quantum well of 3nm width. Then, tow regions of p-AlGaN and p-GaN with 100nm and 500nm, respectively. Cathode and anode are connected on top and bottom of structure, respectively. Figure 10b demonstrates the structure designed in Atlas program. To better indicate the quantum well layer, we have expanded the figure, and it is showed in red layer (figure 10c).



(a)



(b)



(c)

Figure10: Single quantum well LED

3.2.2 The mesh

Mesh plays an important role in obtaining good simulations. This must be done with the greatest care to guarantee the reliability of the results. The numerical method used to solve physical equations is the finite element method. Its basic principle is the finite element discretization of the equations to be treated. The choice of mesh should be made in such a way as to have a trade-off between speed of execution and accuracy of the results, as a thick mesh produces a quick simulation, but the results are less precise. Whereas a fine mesh produces slower simulation, but more precise results. So the fine mesh is more interesting from a result point of view in the simulation. Thus, the mesh designed for our structure is shown in the figure below.

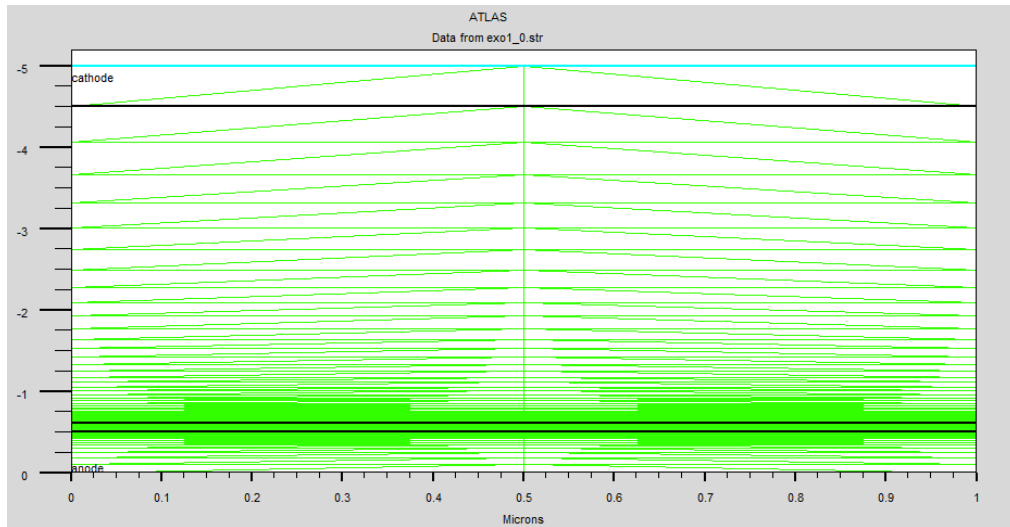


Figure 11: Single quantum well LED mesh

3.2.1 Simulation parameters of LED :

To simulate a device, you must specify the parameters of the materials used to manufacture that device such as the gap energy E_g (eV), electron mobility (cm^2/Vs), the lifetimes of electrons and holes (τ_{n0} and τ_{p0}) and Auger Recombination of electrons and holes (aug_n and aug_p). These parameters are defined and grouped in Table 1

Parameters	GaN	AlGaIn	InGaIn
Bande gab E_g (eV)	3.42	3.77	2.51
Electronic affinity (eV)	4.23	3.98	4.87
Mobility (cm^2/Vs)	$\mu_{n0}=100$ and $\mu_{p0}=10$	10	100
Lifetime of electrons and holes τ_{n0} and τ_{p0} (ns)	10^{-9} 10^{-9}	10^{-9} 10^{-9}	10^{-9} 10^{-9}
Auger Recombination aug_n and aug_p	10^{-34} 10^{-34}	10^{-34} 10^{-34}	10^{-34} 10^{-34}

Table 1: Simulation parameters of single quantum well LED

3.3 Results and discussion

In order to demonstrate the high performance of single quantum well LED structure in comparison to that of conventional LED, both designs are simulated and studied using Silvaco-Atlas software. Figure 12 shows J-V characteristics of both conventional and single quantum well LEDs. This latter is simulated with 3nm well width. It is clear that the single quantum well LED structure indicates high current density compared to that of simple LED, where a threshold voltage is 2.8V and 3.1V for SQW and conventional LED, respectively. This is can be explained by the number of carriers which can be confined and captured in case of SQW resulting in radiative recombination.

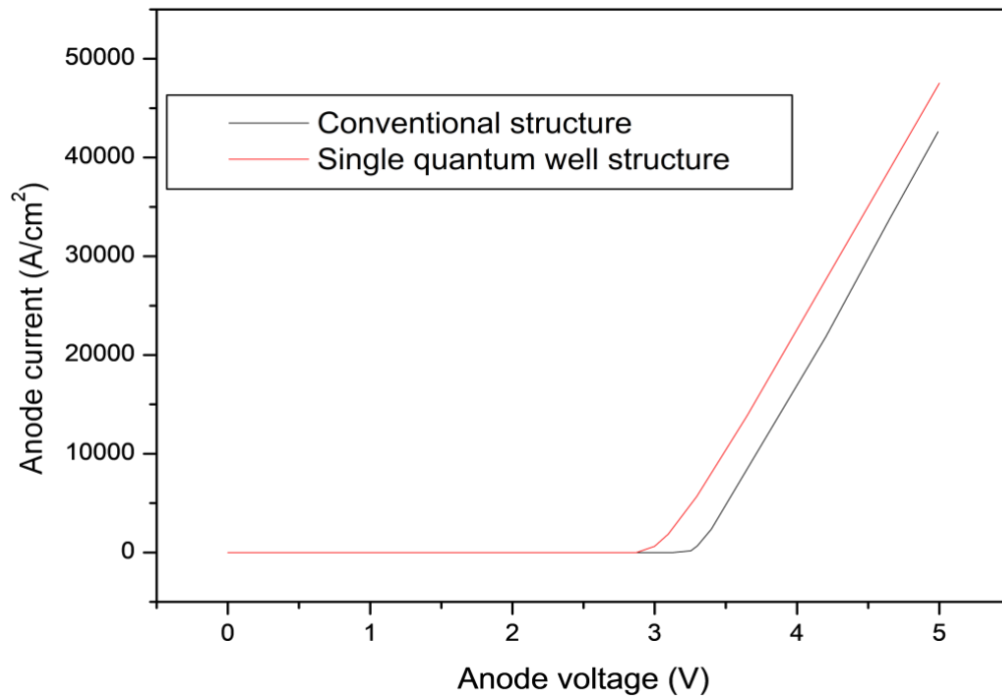


Figure 12: J-V characteristics of SQM and conventional LEDs

Figure 13 illustrates the variation of luminescent power as a function of anode voltage. It presents linear increasing of luminescent power for both structures. Accordingly, the high current delivered by SQW design resulting in high luminescent power compared to the conventional design.

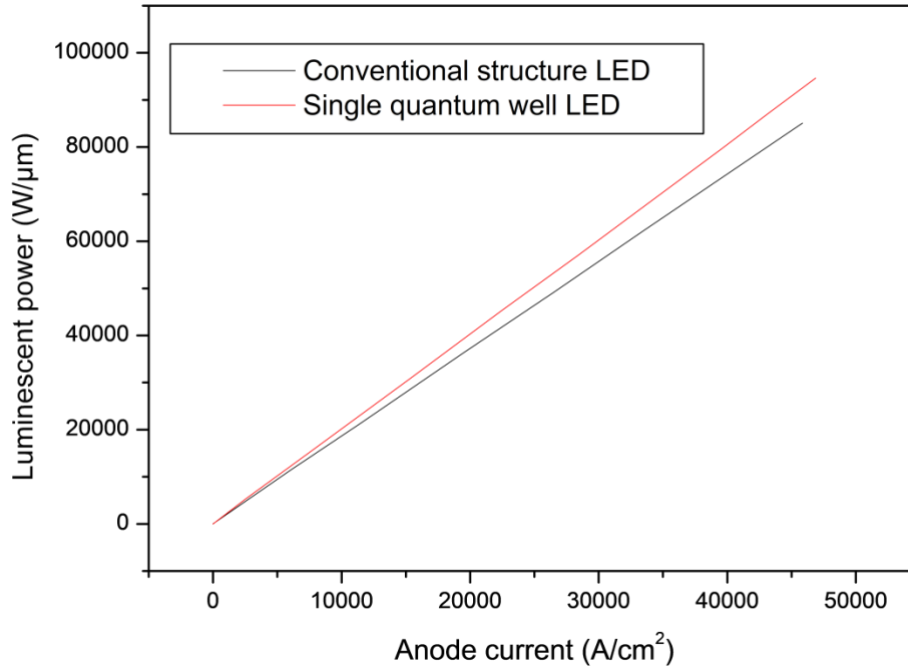


Figure 13: Variation of Luminescent power versus anode current

Figure 14 plots I-V characteristics of single quantum well LED with different well width. From the figure, it is observed that all characteristics are almost present the same variation, but there is a little difference between them. The value of 47519 A/cm² is observed in case of 4nm well-width, 47523 A/cm² and 47558 A/cm² are for 3nm and 2nm well-width, respectively. The decreased current in case of 4nm well-width is due to the more separation of hole and electron wave functions, resulting in less hole and electron recombination. However, when the quantum well is very thin, the carrier recombination is favored and thus the overflow increases. Consequently, the luminescent power is increased in case of 2nm compared to 3nm and 4nm well-width which can be illustrated in figure 15.

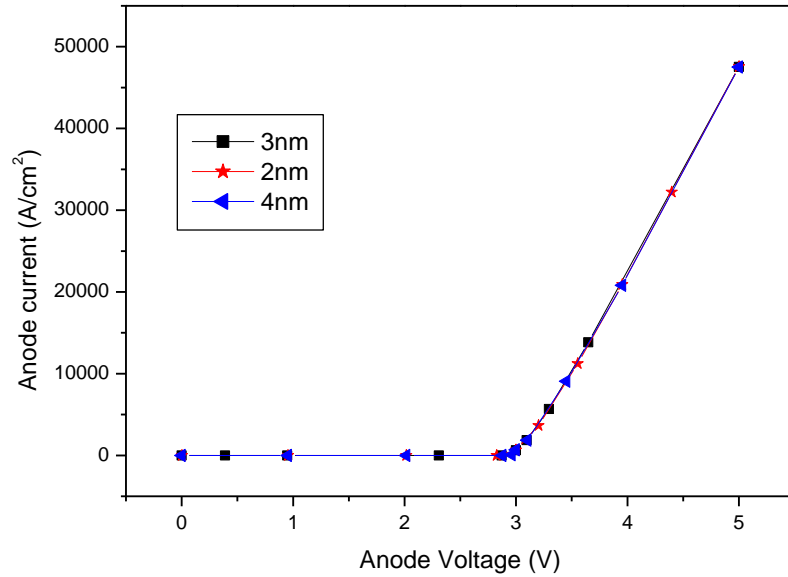


Figure 14: I-V characteristics of SQW LED for different well-width

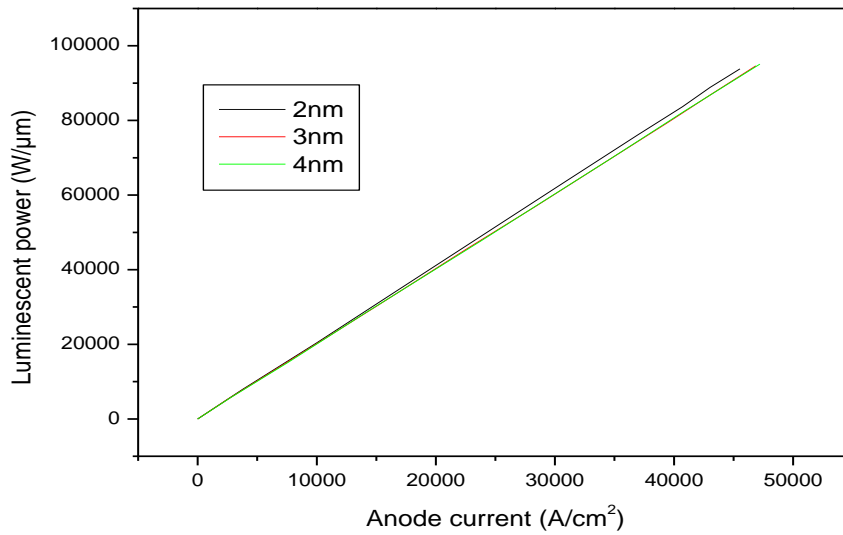


Figure 15: Luminescent power versus anode current with diverse well-width

Conclusion

In this chapter, we have simulated and studied the single quantum well LED (SQW) design using Silvaco-atlas software. This latter has been compared to the conventional structure in order to show the high performance provided by the SQW. It is evident that the single quantum well LED structure indicates high current density and high luminescent power compared to that of standard LED structure. In addition, the influence of well-width on SQW design has been modeled and studied. The obtained results demonstrate that the value of 47519 A/cm^2 is observed in case of 4nm well-width, 47523 A/cm^2 and 47558 A/cm^2 are for 3nm and 2nm well-width, respectively. Clearly, the well-width of 2nm provides better performance compared to that of 3nm and 4nm.

General conclusion:

General conclusion:

The light emitting diode is an increasingly used component in various fields such as lighting, television screens, computer screens or decoration. It can replace traditional light sources. In this work, we briefly presented a theory of light emitting diode and its operation principle. Then, different characteristics and their application in diverse domains are also given.

Different types of LED such as organic LED, homojunction LED, and heterojunction LED are described. However, the structure that we have simulated is single quantum well (SQW) light-emitting diode based on InGaN material; the well is placed between two layers of n-GaN and p-AlGa_N. This sandwich traps both electrons and holes in the active region, thereby increasing the rate of radiative recombination. We extracted the main electrical characteristics such as IV and PV by Atlas simulation software. Single quantum well diode has better performance causes the light emission of the LED diode to come only from the Quantum well. Thus the good distribution of the light emission in LED diode is due to the homogeneous distribution of the charges, in quantum wells because the rate of radiative recombination in the quantum wells is directly proportional to the product of the concentration of the holes and of the electrons in the well.

The single quantum well LED (SQW) design has been compared to the conventional structure in order to show the high performance provided by the SQW. The obtained results indicate that the single quantum well LED structure shows high current density and high luminescent power compared to that of standard LED structure. In addition, the influence of well-width on SQW design has been modeled and studied. It is evident that the value of 47519 A/cm² is observed in case of 4nm well-width, 47523 A/cm² and 47558 A/cm² are for 3nm and 2nm well-width, respectively. Clearly, the well-width of 2nm provides better performance compared to that of 3nm and 4nm.