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Réalisé par : Hamdaoui Mohammed abdel basset
Debba Ahmed Badr Eddine
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Contribution à l'étude par simulation d'une diode électroluminescente (LED) à base de InGaN/GaN à multi puits quantiques par TCAD SILVACO-

Jury de soutenance :

Nom et Prénom	Grade	Qualité
Selmane Naceur	MCA	Encadrant
Cheknane Ali	Pr	Co-Encadrant
Birane Mouhoub	MCA	Président
Vilboi Leila	MAA	Examinateur

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Dedication

All praise to Allah the Almighty, who has guided us to this, and we would not have reached it if Allah had given us grace
WE dedicate this humble work to our dear mothers and our dear fathers, may Allah protect them.
It is to us who remained standing and worked hard for our education to complete this work near or far and to our family members.
To all our relatives and all our friends without exception.
To our dear teachers and to all our classmates.
Finally, we ask Almighty Allah to make this work a benefit for all the stuck students who are about to graduate.

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We are indebted to our parents and all of our families for their love, sacrifice, and patience.

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Valence band	**Ev**
Conduction band	E_C
The band gap	E_G
Fermi level	E_F
Silicon	Si
Germanium	Ge
Light emitting diodes	LEDs
Full-color displays	LCD
Gallium-nitride	Gan
Aluminum-nitride	AlN
Cubic close-packed	CCP
Zinc sulfide	ZnS
Close packing structure	HCP
Photoluminescence	PL
Cathode luminescence	CL
Metal organic chemical vapor deposition	MOCVD
Indium gallium nitride	InGaN
Metal–oxide–semiconductor field-effect transistor	MOSFET
Ultraviolet	UV
Infrared radiation	IR
Terawatt hour	TWh
Volts	V
Ampere	A

Watt	W
Tension direct	V_F
Planck's constant	H
The frequency	Y
The speed of light	C
The wavelength	Λ
Carrier densities in the junction,	n ; p
Carrier densities at thermodynamic equilibrium	n_0 ; p_0
Spontaneous recombination coefficient	B
The diffusion constants of the electron-holes	Dn, p
The concentrations of donors	ND
Duration of the generated pulse	T
Period of the signal	T
Recessed Architectural Linear	RAL
Brightness index number	BIN
Simple heterostructure	SH
Quantum well	QW
Single Quantum well	SQW
Multiple Quantum well	MQW
Technology Computer-Aided Design	TCAD
Virtual Wafer Fab	VWF
Two dimensions	2D
Three dimensions	3D
Electron Blocking Layer	EBL

Chapter I

Introduction of Semiconductors and III-nitrides

I.1 Introduction

While studying electrical engineering, most topics revolve around these three types of materials conductor, insulator, and semiconductor.

Conductors are materials that possess high conductivity and low resistivity which allows them to conduct electricity. Gold, copper, silver, etc. are few conducting materials.

On the other hand, insulators are materials that possess low conductivity and slightly high resistivity due to which they aren’t able to conduct electricity. Examples of insulating materials are glass, rubber, quartz, etc.

Where the semi-conductor is the median type of material. Because neither it is a good conductor nor a good insulator. Where at absolute temperature it acts as an insulator but at room temperature, its conductivity is lower than the conductor and higher than the insulator. This makes it electrically conducting at room temperature.

I.2 what are Semiconductors?

Semiconductors are the materials which have a conductivity between conductors (generally metals) and non-conductors or insulators (such as ceramics). Semiconductors can be compounds such as gallium arsenide or pure elements, such as germanium or silicon. Physics explains the theories, properties and mathematical approach governing semiconductors. [01]

Semiconductors are employed in the manufacture of various kinds of electronic devices, including diodes, transistors, and integrated circuits. Such devices have found wide application because of their compactness, reliability, power efficiency, and low cost. As discrete components, they have found use in power devices, optical sensors, and light emitters, including solid-state lasers. They have a wide range of current- and voltage-handling capabilities and, more important, lend themselves to integration into complex but readily manufacturable microelectronic circuits. They are, and will be in the foreseeable future, the key elements for the majority of electronic systems, serving communications, signal processing, computing, and control applications in both the consumer and industrial markets. [02]

I.2.1 Examples of Semiconductors Materials

Gallium arsenide, germanium, and silicon are some of the most commonly used semiconductors. Silicon is used in electronic circuit fabrication and gallium arsenide is used in solar cells, laser diodes, etc.

I.2.2 Properties of Semiconductors

Semiconductors can conduct electricity under preferable conditions or circumstances. This unique property makes it an excellent material to conduct electricity in a controlled manner as required.

Unlike conductors, the charge carriers in semiconductors arise only because of external energy (thermal agitation). It causes a certain number of valence electrons to cross the energy gap and jump into the conduction band, leaving an equal amount of unoccupied energy states, i.e. holes. Conduction due to electrons and holes are equally important. [03]

Resistivity: 10^{-5} to 10^{6} Ωm.

Conductivity: 10^{5} to 10^{-6} mho/m.

Temperature coefficient of resistance: Negative.

Current Flow: Due to electrons and holes.

I.3 Band Theory for Semiconductors

I.3.1 Energy Band Gap in Semiconductors

Every solid has its own characteristic energy-band structure. This variation in band structure is mainly responsible for the wide range of electrical characteristics that are observed in various materials. In the case of semiconductors and insulators, the electrons are confined to a number of bands of energy and forbidden from other regions. [04]

The term band gap definition is, it is the energy difference that is present between the top of the valence band and the bottom of the conduction band. Electrons that are able to jump from one band to another band. However, in order for an electron to jump from the state of the valence band to a conduction band, then it requires a specific minimum amount of energy for the transition. The required energy differs from the different materials. Electrons can gain enough energy to jump into the conduction band by absorbing either a “phonon or heat” or a “photon of light”.

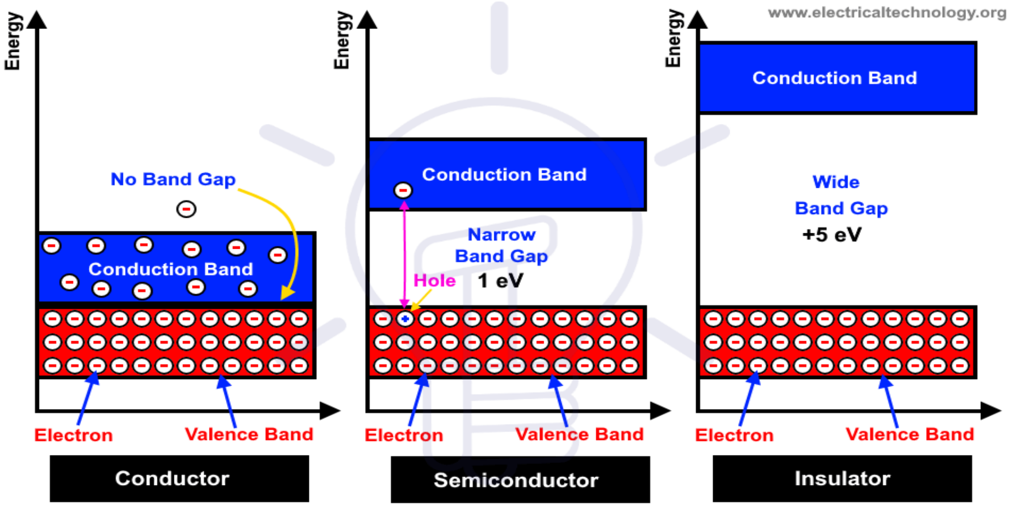

Figure I.1: Difference between Conductor, semiconductor and insulator.

The band gap of a semiconductor is the minimum energy required to excite an electron that is stuck in its bound state into a free state where it can participate in conduction. The band structure of a semiconductor gives the energy of the electrons on the y-axis and is called a "band diagram". The lower energy level of a semiconductor is called the "valence band" (EV) and the energy level at which an electron can be considered free is called the "conduction band" (EC). The band gap (EG) is the gap in energy between the bound state and the free state, between the valence band and conduction band. Therefore, the band gap is the minimum change in energy required to excite the electron so that it can participate in conduction.

I.3.2 Conduction Band, Valence Band and Fermi Level in Semiconductors

- **Valence Band:** The energy band involving the energy levels of valence electrons is known as the valence band. It is the highest occupied energy band. When compared with insulators, the bandgap in semiconductors is smaller. It allows the electrons in the valence band to jump into the conduction band on receiving any external energy.
- **Conduction Band:** It is the lowest unoccupied band that includes the energy levels of positive (holes) or negative (free electrons) charge carriers. It has conducting electrons resulting in the flow of current. The conduction band

possesses high energy level and is generally empty. The conduction band in semiconductors accepts the electrons from the valence band.

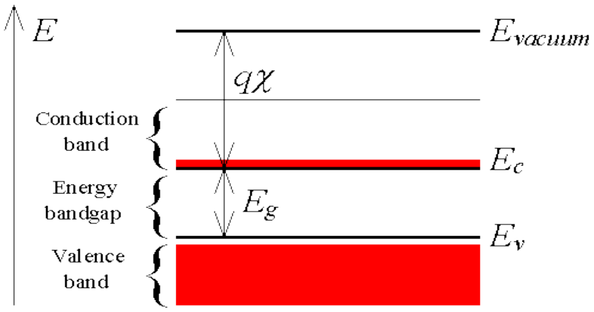

Figure I.2: band gap diagram.

- **Fermi Level:**

Fermi level (denoted by E_F) is present between the valence and conduction bands. It is the highest occupied molecular orbital at absolute zero. The charge carriers in this state have their own quantum states and generally do not interact with each other. When the temperature rises above absolute zero, these charge carriers will begin to occupy states above Fermi level.

In a p-type semiconductor, there is an increase in the density of unfilled states. Thus, accommodating more electrons at the lower energy levels. However, in an n-type semiconductor, the density of states increases, therefore, accommodating more electrons at higher energy levels. [05]

I.4 Types of semiconductor

I.4.1 Intrinsic

A very pure material is used to make an intrinsic semiconductor. Also, it is made up of only a single element. Silicon, germanium, tellurium, boron, etc are various elements but silicon (Si) and germanium (Ge) are the most widely used elements.

A hole-electron pair is formed when the temp. rises and the electron moves to the conduction band leaving a hole in its place. These hole and electron pair is responsible for the conduction of electricity in the intrinsic semi-conductor.

I.4.2 Extrinsic

Extrinsic are those in which some foreign impurities are added into a pure semiconductor. It can be further divided into two types one is N-type or donor semiconductor and the other is P-type or acceptor semiconductor.

An extrinsic semiconductor is one that is doped with a specific impurity in order to improve the conducting properties. This makes the semiconductor suitable for electronic applications like diodes, transistors etc. Depending on the kind of impurities added to the semiconductor it becomes either p-type or n-type.

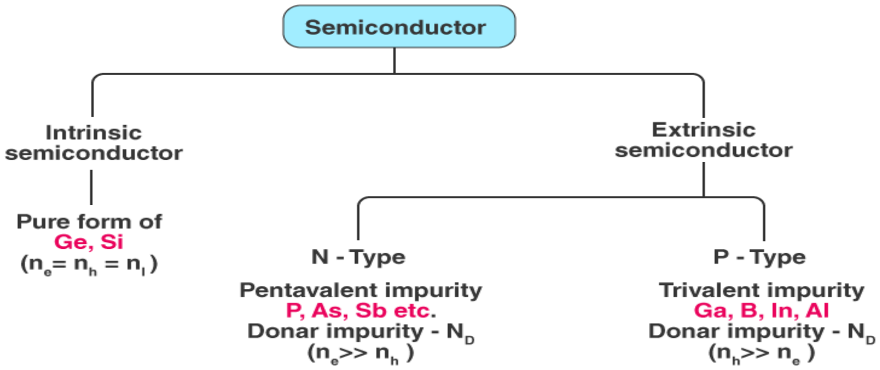

Figure I.3: Classification of Semiconductors.

I.4.3 Difference Between Intrinsic and Extrinsic Semiconductors

Table I.1: Difference between Intrinsic and Extrinsic Semiconductors

Intrinsic Semiconductor	**Extrinsic Semiconductor**
Pure semiconductor	Impure semiconductor
Density of electrons is equal to the density of holes	Density of electrons is not equal to the density of holes
Electrical conductivity is low	Electrical conductivity is high
Dependence on temperature only	Dependence on temperature as well as on the amount of impurity
No impurities	Trivalent impurity, pentavalent impurity

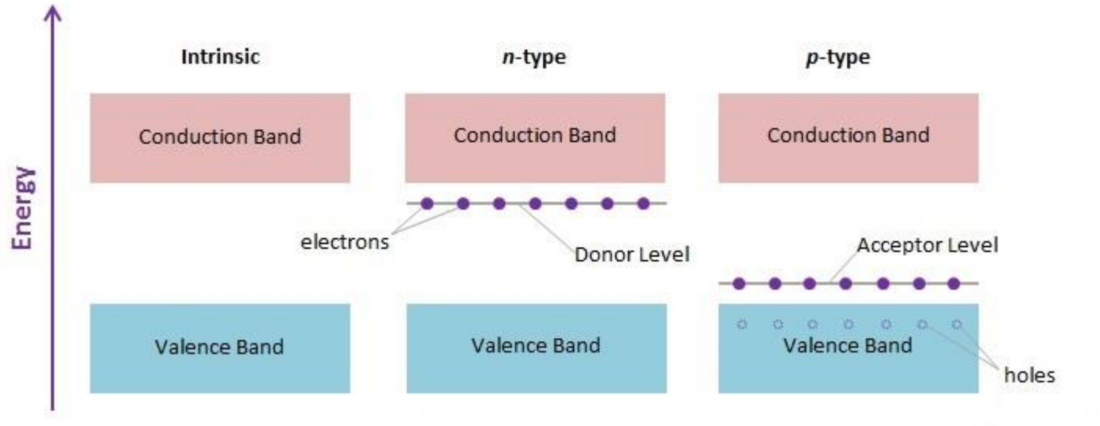

Figure I.4: Energy bands in intrinsic, n-type and p-type semiconductors.

I.5 what is p-type and n-type semiconductor?

In a p-type semiconductor, trivalent impurity from the III group elements is added as the impurity. Trivalent impurities like Aluminium, Indium and Gallium are added to the intrinsic semiconductor. The trivalent impurities added provides extra holes known as the acceptor atom. The majority carriers in a p-type semiconductor are holes.

In an n-type semiconductor, pentavalent impurity from the V group is added to the pure semiconductor. Examples of pentavalent impurities are Arsenic, Antimony, Bismuth etc. The pentavalent impurities provide extra electrons and are termed as donor atoms. Electrons are the majority charge carriers in n-type semiconductors. [06]

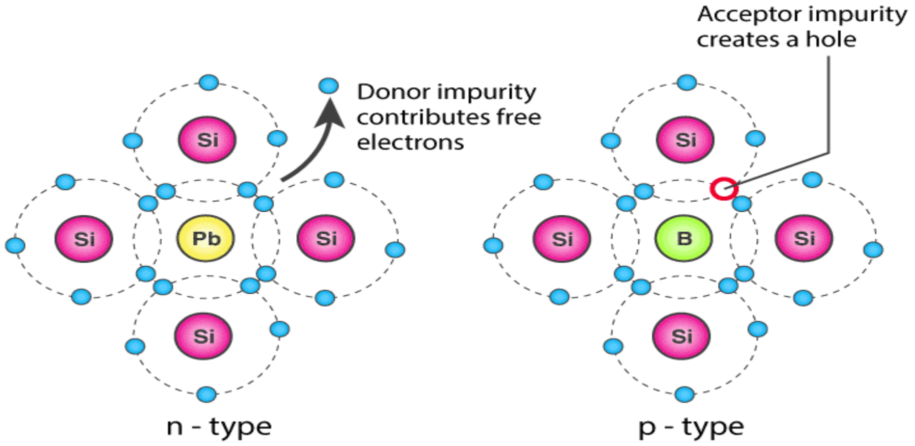

Figure I.5: extrinsic semiconductor crystalline (p-type and n-type).

I.5.1 Difference Between p-type and n-type Semiconductor

- **Dopants:**

In p-type semiconductor, the dopants are Group-III elements.

In n-type semiconductor, the dopants are Group-IV elements.

- **Dopant Behaviour:**

In p-type semiconductor, the dopant atoms are acceptors: they take electrons and create holes in the valence band.

In n-type semiconductor, the dopant atoms act as donors: they donate electrons which can easily reach the conduction band.

- **Majority Carriers:**

In p-type semiconductor, the majority carriers are holes which move in the valence band.

In n-type semiconductor, the majority carriers are electrons that move in the conduction band.

- **Majority Carriers Movement:**

In p-type semiconductor, the majority carriers move in the direction of conventional current (from higher to lower potential).

In n-type semiconductor, the majority carriers move against the direction of conventional current.

I.6 Band gap Types

I.6.1 Direct and indirect band gaps

In semiconductor physics, the band gap of a semiconductor is always one of two types, a direct band gap or an indirect band gap.

The minimal-energy state in the conduction band and the maximal-energy state in the valence band are each characterized by a certain crystal momentum (k-vector) in the Brillouin zone. If the k-vectors are the same, it is called a "direct gap". [07]

If they are different, it is called an "indirect gap".

The band gap is called "direct" if the momentum of electrons and holes is the same in both the conduction band and the valence band; an electron can directly emit a photon. In an "indirect" gap, a photon cannot be emitted because the electron must pass through an intermediate state and transfer momentum to the crystal lattice.

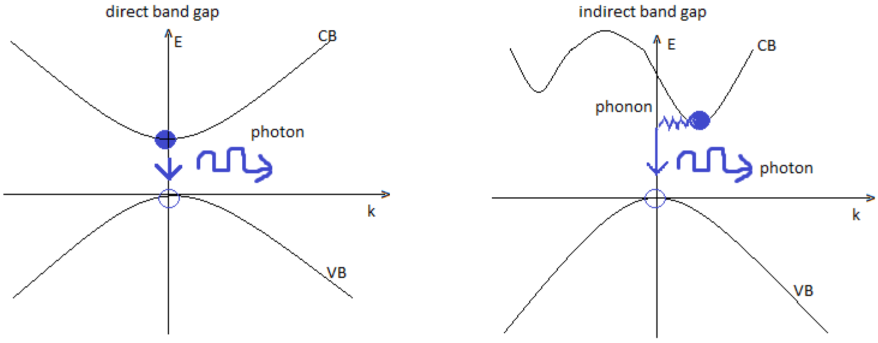

Figure I.6: Comparison of direct and indirect semiconductor band gaps.

For most optoelectronic devices such as light emitting diodes (LEDs), laser diodes, and photodetectors, a direct bandgap is essential for efficient device operation. This is because the optical emission processes in a semiconductor with an indirect bandgap require phonons for momentum conservation. The involvement of the phonon makes this radiative process much less likely to occur in a given time span, which allows non-radiative processes to effectively compete, generating heat rather than light. Therefore semiconductors with an indirect bandgap are not suitable for efficient LEDs.

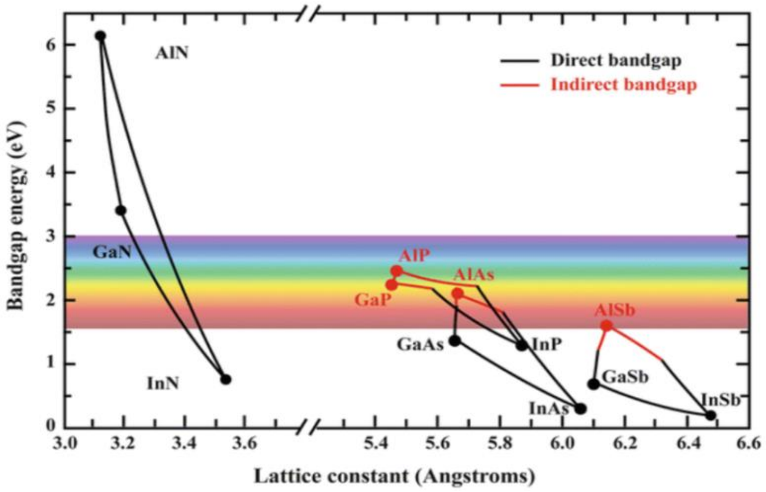

Figure I.7: Bandgap energy in eV of the most important binary semiconductors versus their lattice constant at 300 K. [09].

I.7 Advantages of semiconductor

The semi-conductor used in several devices such as a diode, transistor, etc. has many advantages.

- The devices have a compact size and lightweight
- They are very cheap.
- They are resistive to shock and vibrations.
- Their operating frequency is high.
- They work for a long period if used within the permissible limit of temperature and frequency.

I.8 Application of semiconductor

Day by day with the increase in technology semiconductor requirement is also going to improve. As per industry demands many new devices are discovered in nowadays with the help of semiconductor materials. Without transistor and integrated circuits, our modern life would be very difficult.

The properties of semiconductor materials make possible numerous technological wonders, including transistors, microchips, solar cells, and LED displays. With the microprocessor, we can control the operation of car, trains and space vehicles. The microprocessor is made up by numerous transistor and other controlling devices which made up by the semiconductor material. [08]

I.9 Ill-nitrides

Wide bandgap Ill-nitrides, including (AI,Ga,In)-N, have seen enormous success in their development especially in the latest stages of the 20th century. Many substantial problems had to be overcome before these materials could constitute useful devices. High density of dislocations due to the lack of lattice-matched substrates and low doping efficiency were the most challenging problems that researchers in this area had to face. At the beginning, it was hard to believe that a material with a dislocation density in the order of 10^8 - 10^{10} cm^{-2} would become the building block of many viable devices. However, thanks to the hard work of researches in this field, today blue/violet light-emitting diodes and laser diodes based on (Al,In,Ga)-N have been successfully commercialized. Blue/green LEDs have already found their market in full-color LCD displays and traffic lights, while blue LDs are expected to shortly replace red lasers in the current CD/DVD read/write systems. The unique properties of Ill-nitrides lead to a range of applications from optoelectronic devices to high-power electronics. The wide bandgap of GaN makes this material suitable not only for light emitting source but also for high-temperature applications. GaN and its alloys have the potential to form high power electronics such as transistors or thyristors.. Due to the polar nature of the Ga-N bond, GaN does not possess inversion symmetry. Thus, when GaN is subject to an alternating electric field, the induced polarization is not symmetric. This property of GaN can be used in non-linear optics applications such as second-harmonic generation [10]. The same lack of inversion symmetry results in a huge piezoelectric field. There are some other conceivable applications for Ill-nitrides such as surface acoustic wave generation [11], acousto-optic modulator [12], and devices that utilize negative electron affinity [13].

The most commonly used III-nitride semiconductors are indium-nitride (InN), gallium-nitride (GaN), and aluminum-nitride (AlN). These materials are LED suitable materials for many reasons. Foremost AlN, GaN and InN are direct band gap materials, thus a photon can directly be generated from an electron-hole pair without any phonon involvement. Furthermore the bandgap energies of AlN, GaN, and InN are 6.2, 3.4, and 0.7 eV at room temperature cover the entire visible spectrum from the IR to the deep UV range (see figure 07). Traditional LED materials such as (Al,Ga,In) -arsenides and (Al,Ga,In) -phosfides “only” cover the IR to green -region. III-nitride semiconductors have also strong chemical bonds, which makes the nitrides very stable and resistant to degradation under high electric fields and temperatures.

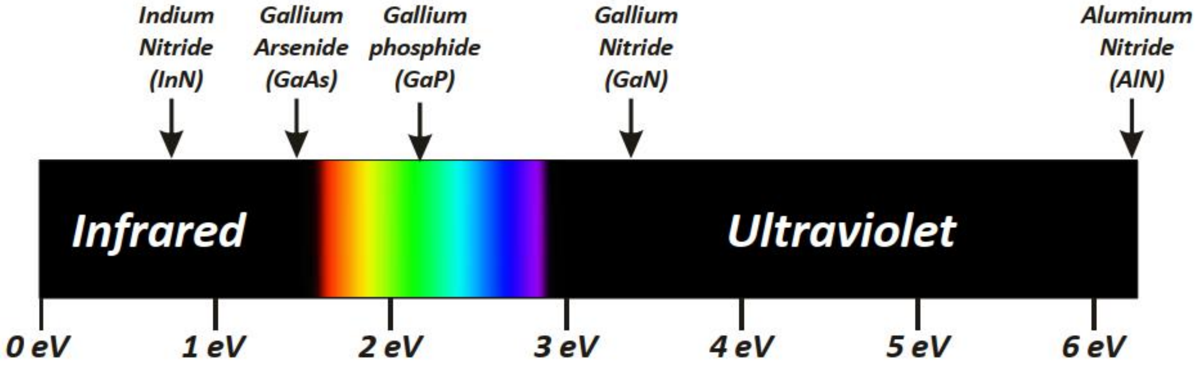

Figure I.8: Band gap energies of some common semiconductors showed in electromagnetic spectra.

I.10 Properties Of III-nitrides

I.10.1 Properties Crystalline

Group III nitrides can have the following crystalline structures: the wurtzite and zinc blende. Under ambient conditions, the thermodynamically stable structure is wurtzite for bulk AlN, GaN, and InN. The zinc blende structure for GaN and InN has been stabilized by epitaxial growth of thin films on {011} crystal planes of cubic substrates such as Si, SiC, MgO, and GaAs. In these cases, the intrinsic tendency to form the wurtzite structure is overcome by topological compatibility.

I.10.1.1 Zinc Blende

Zinc blende is the cubic crystals structure shown by zinc sulfide (ZnS). The structure has a diamond-like network. It is a thermodynamically more favoured structure than the other form of zinc sulfide. However, it can change its structure upon changing the temperature. For instance, zinc blende can become wurtzite if we change the temperature.

We can characterize the zinc blende as a cubic close-packed (CCP) and a face-centred cubic structure. Also, this structure is denser than the wurtzite structure. However, when the temperature increases, the density tends to decrease; therefore, a conversion can take place from zinc blende to wurtzite. Besides, in this structure, the cations (zinc ions) occupy one of the two types of tetrahedral holes present in the structure, and it has four asymmetric units in its unit cell.

I.10.1.2 Wurtzite

Wurtzite is the hexagonal crystal structure shown by zinc sulfide (ZnS). We call this crystal structure hexagonal close packing structure (HCP). We can characterize it by 12 ions in the corners of each unit cell, which creates a hexagonal prism structure.

However, this structure has low thermodynamic stability; thus, it slowly converts into a zinc blende structure. Also, this structure has the cations (zinc ions) occupying one of the two types of tetrahedral holes present in the structure, but it has two asymmetric units in its unit cell.

Table I.2: Lattice parameters of GaN and InN [13].

	InN	GaN
Wurtzite a (A°) c (A°)	3.54 5.70	3.189 5.185
Cubique a (A°)	4.96	4.47

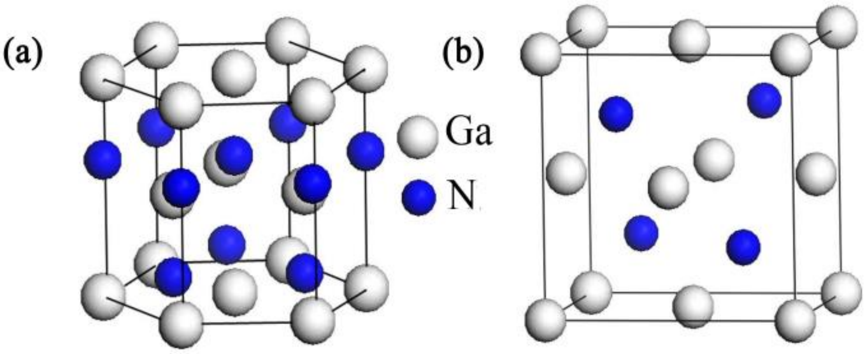

Figure I.9: Crystal structures of: Wurtzite GaN (a); and zinc-blende GaN (b)

I.10.1.3 Difference between Zinc Blende and Wurtzite

Zinc blende and wurtzite are two forms of zinc sulfide. However, the key difference between zinc blende and wurtzite is that zinc blend is cubic, whereas wurtzite has a hexagonal structure. Further, the density of zinc blende is higher than wurtzite.

Moreover, one more significant difference between zinc blende and wurtzite is that the zinc blend has four asymmetric units in its unit cell, while the wurtzite has two asymmetric units. Besides, when considering the thermodynamic stability of these structures, zinc blend is thermodynamically more favoured; thus, the wurtzite structure tends to convert into zinc blend slowly.

Table I.3: Difference Between Zinc Blende and Wurtzite.

	Zinc Blende	**Wurtzite**
Crystal System	Cubic	Hexagonal
Density	High	Low
Asymmetric Units	Has 4 asymmetric units	Has 2 asymmetric units
Stability	Thermodynamically more stable	Thermodynamically less stable

I.11 Electrical properties

I.11.1 Spontaneous polarization

The absence of an inversion center in the wurtzite structure and the strong ionicity of the III-N element bond have major consequences on the physical properties of nitrides. In their state of equilibrium, these materials have a spontaneous polarization. It comes from the fact that the barycentres of the positive charges (Ga, In, Al atoms) and negative charges (nitrogen atoms) do not coincide in space. Thus, there is creation of a dipole in each cell. These dipoles are then added through the structure to give rise to a macroscopic polarization oriented along the direction of growth c [0001].

Table I.4: Values of spontaneous polarization of GaN and InN [15].

	GaN	**InN**
c/a	1.6259	1.6116
P_{sp}(C/m^2)	-0.029	-0.032

I.11.2 Piezoelectric polarization

All III-V compounds, being non-centrosymmetric, are piezoelectric. As far as nitrides are concerned, this piezoelectricity is very important because the III-N bond is strongly polarized, the electrons being essentially located on the nitrogen atom.

Any stress exerted on a solid generates a deformation of this solid and therefore a change of position of the atoms with respect to each other. If this solid is non-centrosymmetric such as GaN, we observe a modification of the dipole moments of the Ga-N bonds linked to the variation of the interatomic distances. This explains the origin of the piezoelectric polarization which varies according to the stress exerted. In the case of heterostructures, the stresses are generated by the lattice mismatch existing between the two materials. The piezoelectric polarization for materials with a wurtzite structure is given by [16].

$$P_{pz} = 2\left[\frac{a(0)-a(m)}{a(m)}\right] * \left[e_{31}(m) - \frac{e33(m)\ c13\ (m)}{c33\ (m)}\right] \qquad (01)$$

Where: e_{31} and e_{33} are the piezoelectric constants.

c 13 and c 33 are the elastic constants.

a(0) and a(m) are the lateral lattice constants at equilibrium and under stress.

I.12 Optical Properties

Nitrides possess direct band gaps from 0.7 eV (InN), through 3.4 eV (GaN) to 6.1 eV (AlN). Hence, they cover the spectral range from infrared (1770nm) through the visible range up to far ultraviolet (about 200 nm) [17].

For a ternary nitride compound AxB1−xN, the energy band gap does not change linearly with the composition x, but it follows a phenomenological expression:

$$E_g{}^{A}x^{B}1-x^{N}\ (x) = xE_g{}^{A} + (1-x)E_g{}^{B} - x(1-x)b \qquad (02)$$

Where b is bowing parameter (in units of eV), defined as the coefficient of the parabolic term. A positive value of b indicates a downward bowing, while a negative b indicates an upward bowing in the dependence of the energy gap Eg on the composition x.

Typically, in nitride compounds, most of the measurements of the energy gap (and hence of the bowing parameter) are performed using emission techniques, such as photoluminescence (PL) and cathode luminescence (CL).

I.13 What is Gallium nitride?

Gallium Nitride is a binary III/V direct bandgap semiconductor that is well-suited for high-power transistors capable of operating at high temperatures. Since the 1990s, it has been used commonly in light emitting diodes (LED). Gallium nitride gives off a blue light used for disc-reading in Blu-ray. Additionally, gallium nitride is used in semiconductor power devices, RF components, lasers, and photonics. In the future, we will see GaN in sensor technology.

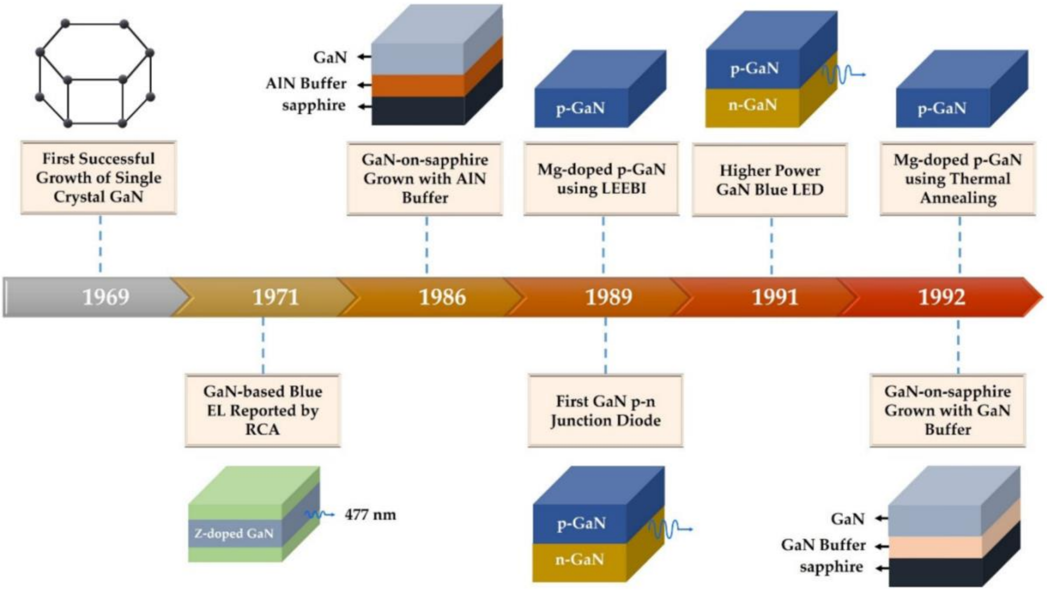

Figure I.10 Timeline of important milestones achieved in the development of the first GaN-based light-emitting p–n junction diode.

In 2006, enhancement-mode GaN transistors, sometimes referred to as GaN FETs, started being manufactured by growing a thin layer of GaN on the AIN layer of a standard silicon wafer using metal organic chemical vapor deposition (MOCVD). The AIN layer acts as a buffer between the substrate and GaN.

This new process enabled gallium nitride transistors to be producible in the same existing factories as silicon, using almost the same manufacturing processes. By using a known process, this allows for similar, low manufacturing costs and reduces the barrier to adoption for smaller transistors with much improved performance.

To further explain, all semiconductor materials have what is called a bandgap. This is an energy range in a solid where no electrons can exist. Simply put, a bandgap is related to how well a solid material can conduct electricity. Gallium nitride has a 3.4 eV bandgap, compared to silicon’s 1.12 eV bandgap. Gallium nitride’s wider band gap means it can sustain higher voltages and higher temperatures than silicon MOSFETs. This wide bandgap enables gallium nitride to be applied to optoelectronic high-power and high-frequency devices.

High-brightness GaN light-emitting diodes (LEDs) completed the range of primary colors, and made applications such as daylight visible full-color LED displays, white LEDs and blue laser devices possible. The first GaN-based high-brightness LEDs were using a thin film of GaN deposited via MOCVD on sapphire. Other substrates used are zinc oxide, with lattice constant mismatch only 2%, and silicon carbide (SiC).

I.13.1 Gallium Nitride Properties

GaN is a very hard, mechanically stable material with large heat capacity. In its pure form it resists cracking and can be deposited in thin film on sapphire or silicon carbide, despite the mismatch in their lattice constants. GaN can be doped with silicon (Si) or with oxygen to N-type and with magnesium (Mg) to P-type, however the Si and Mg atoms change the way the GaN crystals grow, introducing tensile stresses and making them brittle. "There are a huge number of defects in gallium nitride compounds -- a hundred million to ten billion per square centimeter."

The wide band-gap behavior of GaN is connected to specific changes in the electronic band structure, charge occupation and chemical bond regions.

Table 1.5: Properties of GaN.

Properties :	
Chemical formula	GaN
Molar mass	83.730 g/mol
Appearance	yellow powder
Density	6.1 g/cm3
Melting point	>1600 °C
Band gap	3.4 eV (300 K, direct)
Electron mobility	1500 cm2/(V·s) (300 K)
Thermal conductivity	1.3 W/(cm·K) (300 K)
Refractive index (nD)	2.429

Table I.6: Structure Properties of GaN.

Structure Properties :	
Crystal structure	Wurtzite
Space group	C6v4-P63mc
Lattice constant	a = 3.186 Å, c = 5.186 Å
Coordination geometry	Tetrahedral

I.13.2 Advantages of gallium nitride

The value proposition for GaN devices consists of four major points:

1- Reduced energy costs – Because GaN semiconductors are inherently more efficient than silicon, less energy is expended as heat, resulting in smaller system sizes and material costs.

2- Higher power density (smaller volume) – Higher switching frequencies and operational temperatures than silicon result in lower cooling requirements, smaller heat sinks, conversion from liquid-cooling to air cooling, eliminating fans and reduced magnetics.

3- Higher switching frequency – The higher switching frequencies for GaN devices allows smaller inductors and capacitors to be used in power circuits. The inductance and capacitance scale down in proportion to the frequency – a 10X increase in frequency produces a 10X decrease in the capacitance and inductance. This can result in an enormous decrease in weight and volume, as well as cost. In addition, higher frequency can result in less acoustic noise in motor drive applications. High frequency also enables wireless power transfer at higher powers, more spatial freedom and bigger transmits to receive airgaps.

4- Lower system cost – While GaN semiconductors are generally higher cost than silicon, system level cost reductions result through the use of GaN by reducing the size/costs of other components such as passive inductive and capacitive circuit elements, filters, cooling, etc. Savings range from 10-20%.

I.14 Indium gallium nitride

Indium gallium nitride (InGaN, $In_xGa_{1-x}N$) is a semiconductor material made of a mix of gallium nitride (GaN) and indium nitride (InN). It is a ternary group III/group V direct bandgap semiconductor. Its band gap can be tuned by varying the amount of indium in the alloy. The ratio of In/Ga is usually between 0.02/0.98 and 0.3/0.7. [18]

Indium gallium nitride is the light-emitting layer in modern blue and green LEDs and often grown on a GaN buffer on a transparent substrate as, e.g. sapphire or silicon carbide. It has a high heat capacity and its sensitivity to ionizing radiation is low (like other group III nitrides), making it also a potentially suitable material for solar cell arrays for satellites.

InN does not mix homogeneously with GaN. In a composition regime between ~ 15% -85% Indiumnitride spinodal decomposition occurs leading to In-rich and Ga-rich InGaN regions or clusters[19].

GaN is a defect rich material with typical dislocation densities [20] exceeding 108 cm-2. Light emission from InGaN layers grown on such GaN buffers used in blue and green LEDs is expected to be low because of non-radiative recombination at such defects [21].

Nevertheless InGaN quantum wells, are efficient light emitters in green, blue, white and ultraviolet light-emitting diodes and diode lasers. In the indium-rich regions, with a lower bandgap than the surrounding material, most electron-hole pairs recombine and by the lower potential energy of these clusters carriers are hindered to diffuse and recombine non-radiatively at crystal defects.

The wavelength emitted, dependent on the material's band gap, can be controlled by the GaN/InN ratio, from near ultraviolet for 0.02In/0.98Ga through 390 nm for 0.1In/0.9Ga, violet-blue 420 nm for 0.2In/0.8Ga, to blue 440 nm for 0.3In/0.7Ga, to red for higher ratios and also by the thickness of the InGaN layers which are typically in the range of 2-3 nm.

However, atomistic simulations results have shown that emission energies have a minor dependence on small variations of device dimensions [22] Studies based on device simulation have shown that it could be possible to increase InGaN/GaN LED efficiency using band gap engineering, especially for green LEDs [23] .

Conclusion:

Semiconductors are an essential component of electronic devices, enabling advances in communications, computing, healthcare, military systems, transportation, clean energy, and countless other applications.

GaN semiconductors have the capability to operate at higher voltages, temperatures and switching frequencies with greater efficiencies compared to existing Si devices. These characteristics not only result in less losses but enables significantly reduced system volume, due to decreased cooling requirements and smaller passive components contributing to overall lower system costs.

Quantum heterostructures are often built from GaN with InGaN active layers.

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Chapter II

Study of Light-emitting diodes (LEDs

II.1 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.

II.2 Light Emitting Diode

II.2.1 Definition of LED (Light Emitting Diode)

A light-emitting diode (LED) is a semiconductor light source that emits light when current flows through it. Electrons in the semiconductor recombine with electron holes, releasing energy in the form of photons. The color of the light (corresponding to the energy of the photons) is determined by the energy required for electrons to cross the band gap of the semiconductor.[01] White light is obtained by using multiple semiconductors or a layer of light-emitting phosphor on the semiconductor device.[02].

The LEDs are extensively used in segmental and dot matrix displays of numeric and alphanumeric character. The several LEDs are used for making the single line segment while for making the decimal point single LED is used.

The following figures also show the practical and theoretical symbol in circulation:

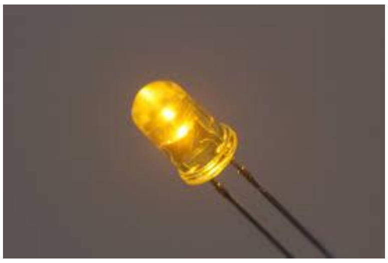

Figure II.1: Practical form LED

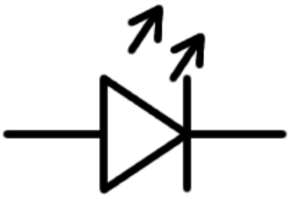

Figure II.2: Theoretical from LED

II.2.2 History of LED

Despite considerable progress in LED technology, it is still in a stage of development. Today we already see devices where one tiny, high-power LED can produce a brighter and better-quality light output than the earlier and the massive arrays containing 96 or more through-the-hole LEDs. However, the electroluminescence was first observed in 1907 by the British experimenter Round of Marconi Labs, using a silicon carbide crystal and a cat's whisker detector.[03]

In 1927, Russian inventor Oleg Losev created the first LED independently [04].

Braunstein of the RCA reported infrared emission from GaAs, GaSb, InP, SiGe, and other semiconductor alloys in 1955 at room temperature 77 K [05].

In 1958, Rubin Braunstein and Egon Loebner patent a green LED made from a lead Antimonide/Germanium alloy. Still, the shift to the industrial application was made by Prof. Nick Holonyak in 1962 with the development of the first practical LED [06].

The first practical visible-spectrum (red) LED was developed in 1962 by Nick Holonyak Jr [07].

This last was red lighting and used only for display applications. The early 70s have seen the appearance of the yellow LED (George Craford, 1972) [08].

In the same year, 1972, the blue and violet valve was discovered (Herbert Paul Maruska) [09].

But the last big step to the worldwide revolution for LED lighting applications was Shuji Nakamura, Isamu Akasaki, and Hiroshi Amano in 1993 with a high-power blue light-emitting diode able to allow white lighting [10].

II.2.3 Economic and energy context of LEDs

Today, from an energy point of view, lighting consumes more than 3,418 TWh of electrical energy per year. This quantity represents approximately 19% of the overall world electricity production and it represents an annual bill of more than 200 billion euros for the consumer. The production of electrical energy for satisfying lighting needs inevitably leads to environmental pollution. Thus, it is estimated that each year, some 1,900 million metric tons of CO2 accompany this energy production by contributing to the greenhouse effect [11].

It is therefore obvious that lighting represents a considerable challenge both energy and economy. However, despite all the advances in science and technology the luminous efficiency of conventional light sources seem to have reached its limits according to Figure I.1. Indeed, ordinary incandescent lamps seem stagnate between 10 and 15 lumens/W, fluorescent lamps maintain an output of 100 lumens/W since the 1970s. On the contrary, the efficiency of light-emitting diodes has not only increases with strong growth. Indeed The LED market does not only increasing since 1993. It is increasing by 21% per year [12]. LEDs have a law of evolution which is called: Haitz's law, it is stated that every decade, the flow light of an LED is multiplied by 30 while its cost is divided by 10. This corresponds to a doubling of the luminous flux every 24 months and a reduction in the price of more than 25% per year [13].

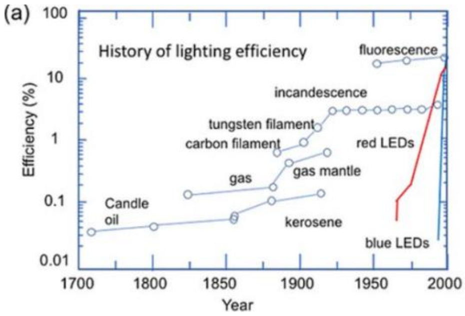

Figure II.3: Evolution of light source efficiency for different technologies.

II.2.4 Main LED materials

The main semiconductor materials used to manufacture LEDs are:

- Indium gallium nitride (InGaN): blue, green and ultraviolet high-brightness LEDs.
- Aluminum gallium indium phosphide (AlGaInP): yellow, orange and red high-brightness LEDs.

- Aluminum gallium arsenide (AlGaAs): red and infrared LEDs.
- Gallium phosphide (GaP): yellow and green LEDs.

II.2.5 Classification of Light Emitting Diodes

Since LEDs are small, robust, reliable and extremely high-efficiency light sources, they are used in almost any application where light is needed. Since the needs are different in each application, the LEDs used also gain variety. One of them is power classification.

LEDs are divided into three different categories according to their power**;** Low-Power, Mid-Power and High-Power.

Power is found mathematically by multiplying voltage and current. For example, a 3 V LED consumes approximately 1 W when driven with a current of 350 mA.

LEDs with power between 0.05 W and 0.10 W are in the Low-Power class. LEDs with a power range of 0.25 W to 0.50 W are known as Mid-Power, those with a power range of 1 W to 3 W are known as High-Power LEDs.

- **Low-Power LEDs** have low brightness, so they are often used as indicator lights. For example, the power light that shows computers running is a Low-Power LED.

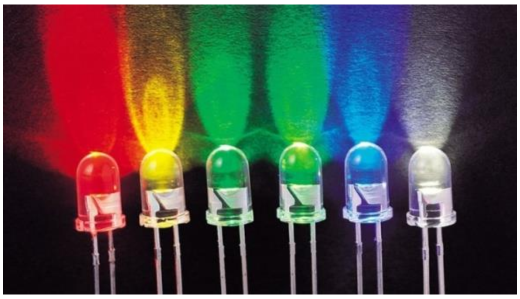

Figure II.4: High-Power LEDs.

- **Mid-Power LEDs** offer high efficiency light with moderately low power consumption. These LEDs, which have a high market share, are used in various applications such as taillights of vehicles as well as indoor and outdoor lighting fixtures. Packaged LEDs such as 2835, 3030, 5050 and 5630 used on LED light strips are Mid-Power LEDs. Mid-Power LEDs are used in almost all E27 or E14 socket LED lamps used in homes.

Figure II.5:High-Power LEDs.

- **High-Power LEDs** are frequently used in new generation lighting applications. With these LEDs with high light output, it is possible to produce high brightness light by using a small number of LED chips. While it was necessary to use hundreds of LEDs to make a 30 W LED lamp in the past, it was sufficient to use 10 LEDs thanks to High-Power LEDs.

Figure II.6: High-Power LEDs.

Power LED definition is generally used for LEDs with a power of 1 W or more. However, as explained above, LEDs (although there is no written international standard defining categories) are basically divided into 3 categories.

The choice of LED in solid state lighting systems affects important parameters such as cost, performance, thermal management and life.

II.3 Working Principle

A light-emitting diode is a two-lead semiconductor light source. It is a p–n junction diode that emits light when activated. When a suitable voltage is applied to the leads, electrons are able to recombine with electron holes within the device, releasing energy in the form of photons. This effect is called electroluminescence, and the color of the light (corresponding to the energy of the photon) is determined by the energy band gap of the semiconductor. [14]

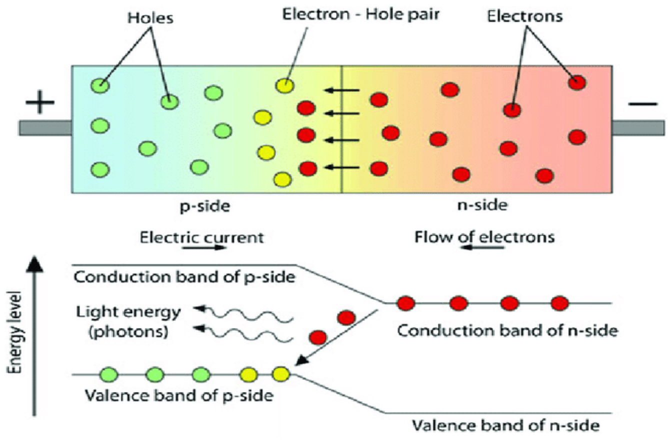

Figure II.7: Working Principle Of LED [15].

II.4 Working Basics in LEDS

- The material used in LEDs is basically aluminum-gallium-arsenide (AlGaAs). In its original state, the atoms of this material are strongly bonded. Without free electrons, conduction of electricity becomes impossible here.
- By adding an impurity, which is known as doping, extra atoms are introduced, effectively disturbing the balance of the material.
- These impurities in the form of additional atoms are able either to provide free electrons (N-type) into the system or suck out some of the already existing electrons from the atoms (P-Type) creating “holes” in the atomic orbits. In both ways the material is rendered more conductive. Thus in the influence of an electric current in N-type of material, the electrons are able to travel from anode (positive) to the cathode (negative) and vice versa in the P-type of material. Due to the virtue of the semiconductor property, current will never travel in opposite directions in the respective cases.
- From the above explanation, it’s clear that the intensity of light emitted from a source (LED in this case) will depend on the energy level of the emitted photons which in turn will depend on the energy released by the electrons jumping in between the atomic orbits of the semiconductor material.
- We know that to make an electron shoot from lower orbital to higher orbital its energy level is required to be lifted. Conversely, if the electrons are made to fall from the higher to the lower orbitals, logically energy should be released in the process.

- In LEDs, the above phenomena is well exploited. In response to the P-type of doping, electrons in LEDs move by falling from the higher orbitals to the lower ones releasing energy in the form of photons i.e. light. The farther these orbitals are apart from each other, the greater the intensity of the emitted light.

Different wavelengths involved in the process determine the different colors produced from the LEDs. Hence, light emitted by the device depends on the type of semiconductor material used.

Infrared light is produced by using Gallium Arsenide (GaAs) as a semiconductor. Red or yellow light is produced by using Gallium-Arsenide-Phosphorus (GaAsP) as a semiconductor. Red or green light is produced by using Gallium-Phosphorus (GaP) as a semiconductor.

II.5 Emission Types

II.5.1 Spontaneous emission

We know that when a quantum mechanical system such as atom, molecule or subatomic particle (electron, proton etc) absorbs extra energy, it goes in a excited energy state. To return to its normal or ground state, it emits the absorbed extra energy in the form of photon at an undetermined time. This unpredictable release of photon energy is known as spontaneous emission.

II.5.2 Stimulated emission

Stimulated emission is the process by which an incoming photon of a specific frequency can interact with an excited atomic electron (or other excited molecular state), causing it to drop to a lower energy level. The liberated energy transfers to the electromagnetic field, creating a new photon with a phase, frequency, polarization, and direction of travel that are all identical to the photons of the incident wave.

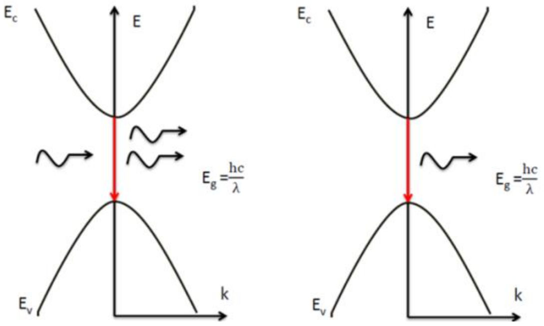

Figure II.8: Stimulated and Spontaneous Emission Mechanisms [16].

II.5.3 Trap emission

Trap emission is a multistep process wherein a carrier falls into defect-related wave states in the middle of the bandgap. A trap is a defect capable of holding a carrier. The trap emission process recombines electrons with holes and emits photons to conserve energy. Due to the multistep nature of trap emission, a phonon is also often emitted. Trap emission can proceed by use of bulk defects [17] or surface defects.[18]

II.6 LED Construction

The structure and construction of Light Emitting Diodes are much different from that of a regular semiconductor signal diode. Light will be emitted from the LED when its PN junction is forward biased. The PN junction is covered by a transparent solid and plastic epoxy resin hemispherical shaped shell body which protects the LED from atmospheric disturbances, vibrations and thermal shock. The PN junction is formed using the lowest band gap materials like Gallium Arsenide, Gallium Arsenide Phosphide, Gallium Phosphide, Gallium Indium Nitride, Aluminum Gallium Nitride, Silicon Carbide etc.

Actually an LED junction does not emit much amount of light so that the epoxy resin body is built in such a way that the photons of light emitted by the junction are reflected away from the surrounding substrate base and are focused through the domed top of the LED, which itself acts as a lens concentrating the larger amount of light. It is the reason why the emitted light appears to be brightest at the top of LED.

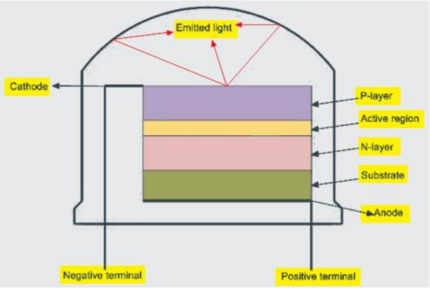

Figure II.9: LED Construction.

Table II.1: Different semiconductors used depending on the color of the light [19].

Spectrum area electromagnetic	**Length wave (nm)**	**Tension direct V_F**	**Semiconductor used**
infrared	$\lambda>780$	$V_F<2.5$	Gallium aluminum arsenide (AlGaAs) Gallium arsenide (GaAs)
Red	$610<\lambda<780$	$1.5<V_F<3$	Aluminum indium gallium phosphorus (AlGaInP) Gallium Aluminum Arsenide (AlGaAs) Gallium Phosphorus Arsenide (GaAsP)
Orange	$590<\lambda<610$	$2<V_F<2.5$	Gallium Phosphorus Arsenide (GaAsP) Gallium phosphorus (GaP) Aluminum indium gallium phosphorus (AlGaInP)
Yellow	$570<\lambda<590$	$1.5<V_F<3$	Aluminum indium gallium phosphorus (AlGaInP) Gallium Phosphorus Arsenide (GaAsP) Gallium phosphorus (GaP)
Green	$500<\lambda<570$	$1.5<V_F<3$	Indium gallium nitride (InGaN) Gallium phosphorus (GaP) Aluminum indium gallium phosphorus (AlGaInP)
bleu	$450<\lambda<500$	$2.5<V_F<4$	Indium gallium nitride (InGaN) Zinc selenide (ZnSe)
Purple	$380<\lambda<450$	$3<V_F<5$	Indium gallium nitride (InGaN) Gallium Nitride (GaN)
Ultra violet	$\lambda<380$	$3<V_F<5$	Indium Gallium Nitride (InGaN) Aluminum gallium nitride (AlGaN)
white	$380<\lambda<780$	$3<V_F<5$	Same as blue or (ultraviolet)

The first light-emitting diode on the market was red. Today the LEDs can produce almost any color. Some even broadcast in infrared or ultraviolet. Nevertheless, any light-emitting diode is by nature, monochromatic and its conversion efficiency depends on the emission wavelength. The following table gives the threshold voltage and the wavelength of the light emitted in depending on the semiconductor used. The higher the energy jump needed to make the diode bandwidth is high, and therefore the threshold voltage is high, the longer the wavelength of the light emitted by the semiconductor is short.

It is defined as the angle of the light emission with respect to the emitting surface. The maximum amount of power, intensity or energy will be obtained in the perpendicular direction with the surface emitting. The angle of light emission depends on the color being emitted and it usually varies between around 80° to 110°.

The color of the light emitted by an LED is not determined by the color of the plastic body enclosing the LED. The enclosing is used to both enhance the light emission and to indicate its color when it’s not driven by an electrical supply. In the recent years, blue and white LEDs are also available, but these are more expensive than the normal standard color LEDs due to the production costs of mixing two or more complementary colors in an exact ratio within the semiconductor compound.

II.7 Properties of Light Emitting Diodes

II.7.1 Physical properties

Light-emitting diodes are based on semiconductor physics, which differs depending on the color you want to obtain.

II.7.2 Gap (gap band)

The energy difference between the top of the valence band and the bottom of the valence band conduction is called the gap; it is a significant quantity of semiconductor materials for which the gap conditions a good number of electronic or optical properties. The family of semiconductor materials can be divided into two groups: materials with direct gap (the maximum of the valence band and the minimum of the conduction band are situated at a value close to the wave vector k on the diagram E(k)) , like most of the compounds from columns III and V of the periodic table, and materials with an indirect gap (the valence band maximum and the conduction band minimum are at distinct values of the wave vector k on the diagram E(k)) .In the context of light-emitting applications, materials with a direct gap are favored or the probabilities of radiative recombinations of the carriers are greater [20].

II.7.3 Recombination Mechanisms in a LED

A light emitting diode is a device that converts electrical energy into optical energy. The supplied electrical energy is used to excite electrons from the valence band to conduction, which upon living for their mean life time tend to fall back and recombine with holes in the valence band to emit the energy. The recombination mechanisms are usually classified as radiative and non-radiative recombinations.

II.7.3.1 Radiative Recombinations

When electron-hole pairs recombine, energy is released. This Energy can be released radiatively or non-radiatively. In the case of recombination radiative, a photon is emitted and the wavelength, therefore the perceived color, depends on the energy of the band gap of semiconductor used, according to the equation

$$h\upsilon = \frac{hc}{\lambda} = Eg \tag{03}$$

Where h is Planck's constant, υ is the frequency, c is the speed of light, λ is the wavelength and Eg is the bandgap energy. There are two types of radiative recombination causing the emission of light at the p-n junction of LEDs. First there is spontaneous recombination, which produces light non-coherent having a spectrum centered around the bandgap energy. The rate of spontaneous recombination is given by the equation:

$$R_{spont} = \beta\ (np - n_0 p_0) \tag{04}$$

Where n and p are the carrier densities in the junction, n_0 and p_0 are the carrier densities at thermodynamic equilibrium while β is the spontaneous recombination coefficient. It is this type of recombination that dominates in light-emitting diodes. At the p-n junction, there can also be stimulated recombinations. The photons emitted in this case are then coherent and quasi-monochromatic. This type of recombination is mainly present in laser diodes and is very low in diodes electroluminescent.

II.7.3.2 Non-radiative recombinations

There are also two other types of recombination inside the junction which are said to be non-radiative because the energy is emitted in the form of crystal lattice vibrations. These recombinations are not desirable in a light-emitting diode because they decrease the light intensity emitted for a given injected current.

- **Shockley-Read-Hall**

The first type of non-radiative recombination: is called Shockley-Read-Hall. It is caused by the presence of defects or impurities in the crystal that create a state intermediate in the forbidden region of the band diagram of the semiconductor. These websites in the crystal matrix can pick up or emit carriers leading to recombinations without photon emission.

$$R^{SRH} = \frac{n.p - n_{i,e}^{2}}{\tau_p.(n+n_1)+\tau_n.(p+p_1)} \tag{05}$$

- **Auger recombination**

It's the second type of non-radiative recombination at the semiconductor junction. It is particularly present when the energy of the band forbidden of the semiconductor is weak. Auger recombination results from capture by a electron or a hole of the energy emitted during a spontaneous or stimulated recombination The carrier which captures the energy then finds itself in an excited state of the conduction band or valence before losing its energy through interactions with the crystal lattice or with other free carriers.

$$R^{AU} = \left(C_n^{AU}.n + C_p^{AU}.p\right).\left(n.p - n_{i,e}^{2}\right) \tag{06}$$

II.7.4 Electrical properties

A light emitting diode is first and foremost a p-n junction. The expression of the currentas a function of the voltage applied in a diode of width A is given by [21].

$$\mathrm{I = qA}\left[\sqrt{\frac{\mathrm{Dp}}{\tau\mathrm{p}}}\ \mathrm{Na} + \sqrt{\frac{\mathrm{Dn}}{\tau\mathrm{n}}}\ \mathrm{Nd}\ \right]\mathrm{e}^{\frac{\mathrm{q(V-VD)}}{\mathrm{KBT}}} \tag{07}$$

Where D_n, p are the diffusion constants of the electron-holes and τn,p are the lifetimes of these minority carriers. N_D and N_A are respectively the concentrations of donors and acceptors. The exponential term shows a sudden increase in current when the voltage V_D is reached, called threshold voltage. The value of D_V depends essentially energy from the bandgap of the semiconductor forming the diode. In its normal operation, an LED is used in direct polarization, that is to say when current flows from the anode to the cathode.

II.7.4.1 LED power supply

The English term "driver" is often used to designate the LED power supply, however this term comes from the world of electronics while in the lighting mode, as the International Commission on Illumination recommends, use the term "ballast". The LED has a current-voltage dependence which is not linear but exponential, so a small variation in voltage generates a large variation in current, and conversely a small variation in current generates a small variation in voltage. The flux being almost proportional to the current, so it is preferable to use a power supply in current rather than voltage to obtain a stable flux. However, many circuits electronics supplying LEDs operate in voltage, that is to say that for a current given in the LEDs, a regulation resistor will be put in series with them and the power supply applies a voltage to the terminals of the assembly. This inexpensive method is inefficient and above all, does not protect the LEDs against a possible runaway which is responsible for premature component failures and can even pose a serious fire problem. This problem can be solved by using a resistor-based regulator. Positive thermal. The resistance increases with the heat, The advantage of this solution lies in the simplicity of the assembly and in its robustness, knowing that its performance is not optimal (around 75%). If we seek to increase the yield of food it must use electronic power supplies (current sources) that we can split into two main families: linear regulations and pulsed regulations [22]

II.7.4.2 Linear regulations

Conventional regulators have low efficiencies (70-75%), but by usings witching systems, their efficiency can reach 90% (even 95% in some cases), which makes them very effective.

II.7.4.3 PWM pulse power supply

It is a pulsed current power supply, otherwise known as PWM (Pulse Width Modulation, modulating the width of current pulses). This pulsating current consists of pulses of fixed amplitude whose duty cycle Rc is varied, expressed:

$$\mathrm{RC} = \frac{\tau}{\mathrm{T}}$$

τ: the duration of the generated pulse, T: the period of the signal.

Driving with PWM is mainly used for power LEDs. Using the PWM on can control the light output of LEDs well. Indeed, the PWM can be implemented for:

- Fix the luminous flux of an LED. In this case the duty cycle is kept constant.

- The "Dimming" effect: varying the light output over time. Here wenote that the duty cycle varies.

II.7.6 Optical properties

II.7.6.1 Directivity of the light beam

Whereas a conventional incandescent bulb emits in almost all the space and very homogeneous way, the beam of a conventional LED is much more directional (angle emission of approximately 10, 20, 30°). The new high-power LEDs have less directional beams emit in emission cones of about 110 - 140°.There are two categories of LEDs depending on the direction of emission:

- LEDs with normal radiation, for which the emission is in the direction perpendicular to the plane of the junction.

- Lateral radiation LEDs for which the emission takes place in a plane parallel to that of the junction [23].

II.7.6.2 Binning

The material of the LED chip determines the wavelength and therefore the color. However, a slight variation in the manufacturing conditions can modify the perceived hue .These differences arise from the fact that it is impossible to precisely control all the production parameters, such as substrate temperature, level variations atomic or the mixture of gases. For this, a selection process is applied after the manufacturing: we talk about BINNING (or chip-to-chip variation). During this process, the LEDs are grouped according to their common properties such as luminous flux, electrical behavior or tint. Each group receives a BIN code. We can say that the BIN code is the color palette of LEDs just like the RAL palette in painting. The maximum security that a manufacturer can offer is the use of a unique BIN in all its LED modules [24].

II.8 Homojunction LED

Homojunctions are made from two blocks of the same nature but of different doping to form a PN junction. Carrier recombination is predominant in the "p" zone, this phenomenon is explained by the fact that the holes have a much lower mobility than electrons and results in the presence of a greater number more electrons (minority carriers) in the “p” zone than holes (minority carriers) in the “n” area. The luminescence is therefore more important on the "p" side; this is the reason for which the LEDs are manufactured with the "p" zone close to the emitting surface. Homojunction technology quickly reaches its limits, because by increasing the level of doping to improve the injection efficiency, we simultaneously increase the impurities which in turn constitute additional centers of non-radiative recombination. Otherwise, in a diode, the photons generated by the luminescent center can be reabsorbed. This Radiation trapping increases rapidly with the level of doping. Get diodes producing several hundred lumens requires the implementation of another technology, that of heterojunction [25].

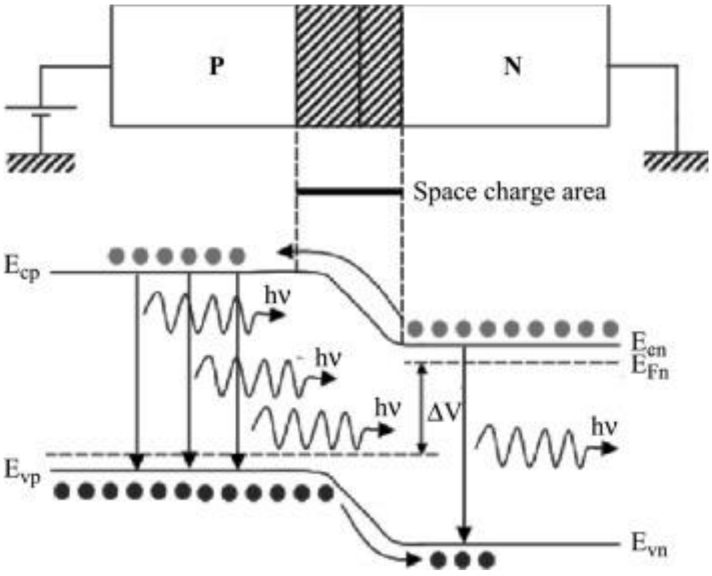

Figure II.10: Band diagram of a PN junction Homojunction.

II.9 Heterojunction LED

The main idea of heterojunction technology is based on the spatial variation of the composition of the semiconductor. These structures, called heterostructures, are assemblies of semiconductors of different chemical compositions also having different energy gaps.

II.9.1 Types of heterojunctions

- **Type I (straddling):** The bandgap of one semiconductor is completely contained in the bandgap of the other one; i.e. $E_C(2) > Ec(1)$ and $E_V(2) < E_V(1)$. The discontinuities of the bands are such that both types of carriers, electrons and holes, need energy (ΔE_C and ΔE_V, resp.) to change from the material with the smaller band gap to the one with the larger gap – the carriers from the other side loose this energy when they cross the junction. Type I heterojunctions are quite common, the important GaAs/AlGaAs system belongs to this kind.
- **Type II (staggered):** The bandgaps overlap, but one ΔE_C or ΔE_V changes sign. The situation with respect to moving carriers from (1) to (2) or vice verse is no longer symmetrical. One kind of carrier gains energy (in the example if electrons move from right to left), the other one needs energy (the holes). The InP/InSb system provides an example.
- **Type III (broken-gap):** The bandgaps do not overlap at all. The situation for carrier transfer is like type II, just more pronounced. The system GaSb/InAs belongs to this type.

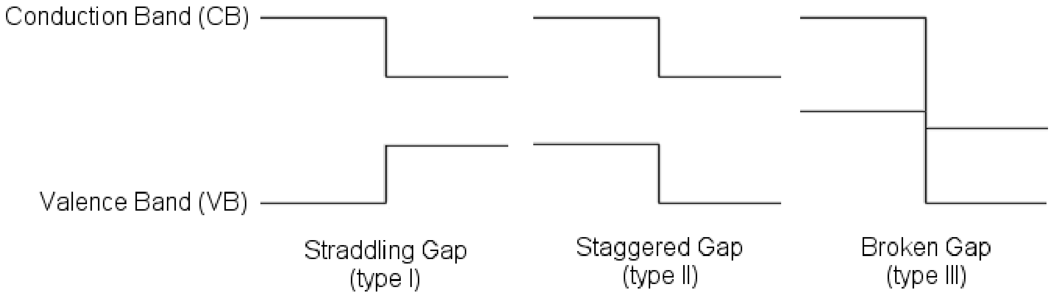

Figure II.11: The three types of semiconductor heterojunctions organized by band alignment.

II.9.2 Simple heterostructure (SH)

In the case of a simple heterostructure (SH), the "p" zone corresponding to the region conduction consists of a semiconductor having an energy gap Eg2 of a value lower than that of the gap of zone "n", Eg1. The discontinuity between the two structures energy amplifies the potential barrier visible by the holes wishing to diffuse towards the region “n”. This shift is equal to EV. For their part, the electrons see a decrease in the potential barrier equal to EC. In this configuration, the ratio between the currents In/Ip increases by a factor proportional to exp (E/kBT), where EV < E < $E_V + E_C$.

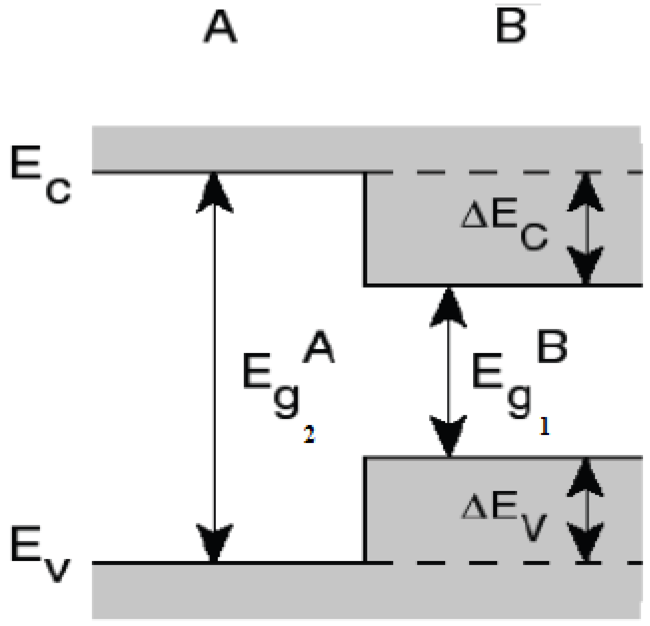

Figure II.12: diagram of a heterojunction.

It is therefore possible to act on the injection efficiency without having to increase the doping level indefinitely. The use of double heterostructures (DH) induces quantum phenomena that modify the energy spectrum of the carriers (confinement quantum) and favor the increase of the efficiency of the diode. So we are talking about LEDs single (SQW) or multiple (MQW) quantum wells [26].

II.9.3 Double heterostructures (DH)

The double heterostructure is a very useful structure in optoelectronic devices and has interesting electronic properties. If one of the cladding layers is p-doped, the other cladding layer n-doped and the smaller energy gap semiconductor material undoped, a p-i-n structure is formed. When a current is applied to the ends of the pin structure, electrons and holes are injected into the heterostructure. The smaller energy gap material forms energy discontinuities at the boundaries, confining the electrons and holes to the smaller energy gap semiconductor. The electrons and holes recombine in the intrinsic semiconductor emitting photons. If the width of the intrinsic region is reduced to the order of the de Broglie wavelength, the energies in the intrinsic region no longer become continuous but become discrete. [27] (Actually, they are not continuous but the energy levels are very close together so we think of them as being continuous.) In this situation the double heterostructure becomes a quantum well.

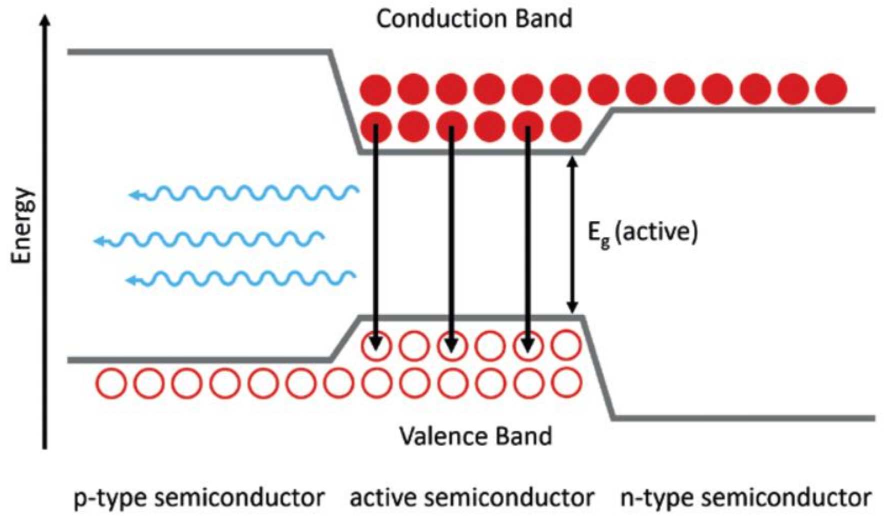

Figure II.13: Working principal of double heterojunction.

II.10 Quantum well LEDs

A quantum well is obtained by growing a layer of a material semiconductor A (typically a few tens of nanometers) between two layers of another semiconductor material B. The latter has an energy gap greater than that of the material A. The discontinuity between the energy bands in the two materials creates a potential barrier that confines the carriers in the quantum well.

The denomination well and barrier comes from the fact that the electrons and the holes originate from the large bandgap barrier material to the potential well at higher mall forbidden band. The well is said to be quantum if its dimensions are sufficiently small (on the order of a nanometer) so that the energy levels in it are quantified. We can then vary the emission wavelength between the bandgap energy of the well and barrier, by changing the width of the well. When an electric voltage is applied to this stack, the charges are injected into the quantum wells, they recombine and their energy difference is released as a photon. The quantum well makes it possible to have better radiative efficiency by concentrating the electrons and holes in a small volume: electron-hole recombinations are then more probable. A single quantum well can be saturated with carriers, which means that at high current the number of photons emitted remains constant above a certain threshold. To overcome this problem, structures with multiple quantum wells are fabricated [28].

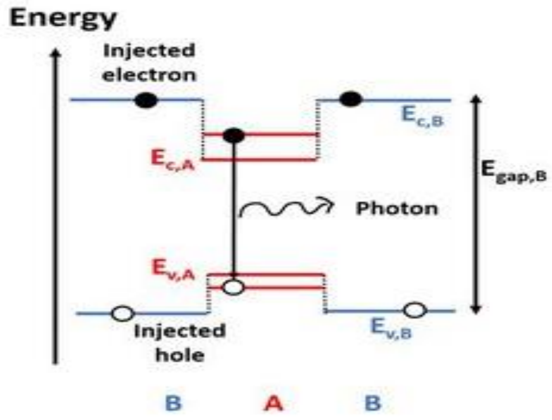

Figure II.14: band diagram of quantum well.

A quantum well is a potential well with only discrete energy values. The classic model used to demonstrate a quantum well is to confine particles, which were initially free to move in three dimensions, to two dimensions, by forcing them to occupy a planar region. The effects of quantum confinement take place when the quantum well thickness becomes comparable to the de Broglie wavelength of the carriers (generally electrons and holes), leading to energy levels called "energy sub bands", i.e., the carriers can only have discrete energy values.

A wide variety of electronic quantum well devices have been developed based on the theory of quantum well systems. These devices have found applications in lasers, photodetectors, modulators, and switches for example. Compared to conventional devices, quantum well devices are much faster and operate much more economically and are a point of incredible importance to the technological and telecommunication industries. These quantum well devices are currently replacing many, if not all, conventional electrical components in many electronic devices [29].

II.10.1 Fabrication

Quantum wells are formed in semiconductors by having a material, like gallium arsenide, sandwiched between two layers of a material with a wider bandgap, like aluminum arsenide. (Other examples: a layer of indium gallium nitride sandwiched between two layers of gallium nitride.) These structures can be grown by molecular beam epitaxy or chemical vapor deposition with control of the layer thickness down to monolayers. Thin metal films can also support quantum well states, in particular, thin metallic over layers grown in metal and semiconductor surfaces. The vacuum-metal interface confines the electron (or hole) on one side, and in general, by an absolute gap with semiconductor substrates, or by a projected band-gap with metal substrates. There are 3 main approaches to growing a QW material system:

- lattice-matched, strain-balanced, and strained Lattice-matched system: In a lattice-matched system, the well and the barrier have a similar lattice constant as the underlying substrate material With this method, the bandgap difference there is minimal dislocation but also a minimal shift in the absorption spectrum.
- Strain-balanced system: In a strain-balanced system, the well and barrier are grown so that the increase in lattice constant of one of the layers is compensated by the decrease in lattice constant in the next compared to the substrate material. The choice of thickness and composition of the layers affect bandgap requirements and carrier transport limitations. This approach provides the most flexibility in design, offering a high number of periodic QWs with minimal strain relaxation.
- Strained system: A strained system is grown with wells and barriers that are not similar in lattice constant. A strained system compresses the whole structure. As a result, the structure is only able to accommodate a few quantum wells [30].

II.10.2 Types of Quantum Well

Quantum well semiconductor LEDs with both single and multiple active layers have been fabricated. Quantum well lasers with one active are called single-quantum-well (SQW) LEDs and LEDs with multiple quantum well active regions are called multiquantum-well (MQW) LEDs. The layers separating the active layers in a multiquantum well structure are called barrier layers. Typical examples of the energy band diagram of both SQW and MQW are schematically represented in Figure.

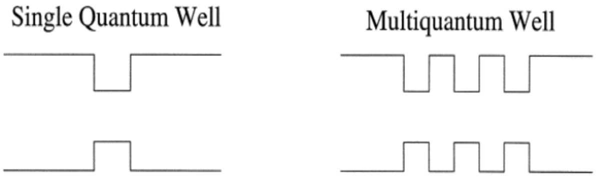

Figure II.15: SQW and MQW Band Diagram.

II.10.2.1 Single quantum well

A quantum emitter is generally defined as a quantum system that is capable of radiative optical transitions. When observing the spontaneous decay of a single excited quantum emitter, the emission of a single photon is expected. When suppressing non-radiative decay mechanisms, they can principally act as 100% efficient single-photon sources. The variety of systems offered by nature allows a multitude of possible experiments and implementations of photonic applications.

A quantum well can be created by sandwiching a single layer of material (let’s call it material A) between two layers of material B, as shown in the drawing on the left-hand side in the figure below. Notice that material B has a larger band gap as compared to material A, $E_g,B>E_g,A$.

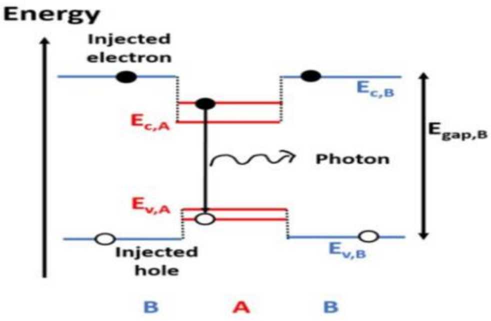

Figure II.16: single quantum-well heterostructures.

II.10.2.2 Multiple Quantum well

In brief, a multiple quantum well (MQW) can be created by stacking layers of materials with different energy band gaps E_g along the z-axis, in an alternating fashion, as shown in the drawing on the left below (A = material A and B = material B). An energy gap is the difference in energy between the conduction Ec band and the valence band Ev [31]. To create a quantum well, the energy gap of material B must be larger than that of material A $E_g,B>E_g,A$. The drawing on the right shows the energy diagram of the quantum well (Take note on the direction of z-axis).

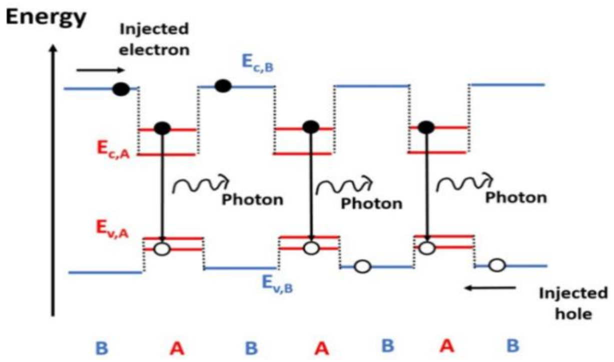

Figure II.17: Multiple quantum-well heterostructures.

A multi quantum well is formed in semiconductors by using a material like gallium arsenide that is allowed to be sandwiched between two layers of aluminium arsenide having a wide band gap.

As shown in the energy diagram on the right, electrons will be injected to the higher energy level (known as conduction band) while holes will be injected to the lower energy level (known as valence band). The quantum wells serve to trap these inserted charge carriers. As holes and electrons are confined within the quantum well, there is a greater chance that they ‘meet with each other’ (wave function overlap). The ‘meeting’ of electrons and holes will result in radiative recombination, where electrons will de-excite from the higher energy level to recombine with holes. Subsequently, packets of energy known as photons are emitted. Depending on the size of the energy gap of a material, different wavelengths (different colors) of light can be emitted.

This design (quantum well) is extremely powerful since it resembles the particle in a box model in quantum mechanics which is well understood [32]. For instance, one knows that the distinct energy levels of the particle within the box is inversely proportional to the width of the box, therefore, in MQW LED, if one varies the thickness of the material A layer, the emission wavelength of a LED can be tuned. In other words, one can change the color of LED by just varying the thickness of material A layer.

One of the most popular LED’s uses GaN as barrier layer (material B) while the well layer (material A) is $In_xGa_{1-x}N$ alloy where the amount of indium in the InGaN alloy is corresponds to the x value. Theoretically, increasing the indium content x allows the color of LED to change from violet to red. However, the cost of doing so is the drop in the crystal quality which then strongly suppress the performance of LED.

Present interest in these III-nitrides materials (e.g. GaN, InGaN, and AlGaN) began when the first long-lived, efficient blue LED was introduced by Nobel laureate Prof. Shuji Nakamura[33] .

In a study, it was found that when 70% of indium was there in InGaN multi quantum well layers, the photoluminescence full-width at half maximum was stronger than in the case of low-indium-content InGaN MQW LED structures. As easy as it can get, with an increasing composition in the MQWs, the optical performance of the LED structures at room temperatures was increased because of the increase in localized energy states which in turn was caused by altering the composition of MQWs.

II.11 The Evolution of the LEDs

LEDs have developed a lot through the years and figure below we represent some of structures:

- The metal-insulator-semiconductor(MIS) structure reported in the 1970s .
- The homojunction-based device reported in the late 1980s.
- The more efficient double heterojunction LED reported in the early 1990s. Since the mid-1990s, the device has been mostly realized with InGaN/GaN.
- Single- quantum-well-based heterostructures.
- Multi-quantum-well-based heterostructures.

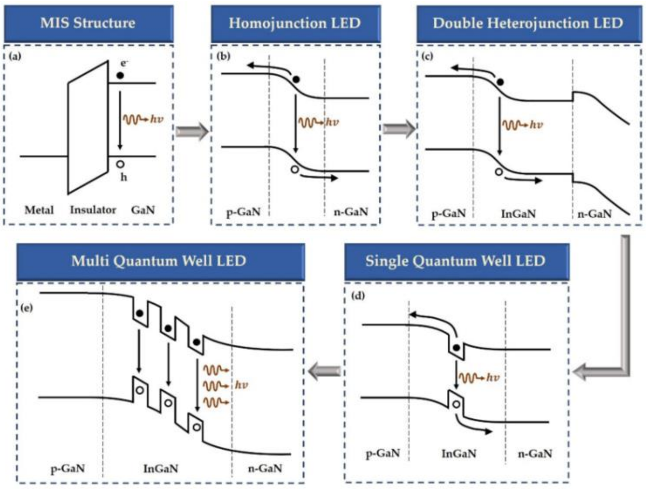

Figure II.18: Energy band diagram of the GaN-based LED.

II.12 Advantages of LEDs

- Very low voltage and current are enough to drive the LED. Voltage range – 1 to 2 volts. Current – 5 to 20 milliamperes.
- Total power output will be less than 150 milliwatts.
- The response time is very less – only about 10 nanoseconds.
- The device does not need any heating and warm up time.
- Miniature in size and hence lightweight.
- Have a rugged construction and hence can withstand shock and vibrations.
- An LED has a lifespan of more than 20 years.

II.13 Disadvantages

- A slight excess of voltage or current can damage the device.
- The device is known to have a much wider bandwidth compared to the laser.
- The temperature depends on the radiant output power and wavelength.

II.14 Applications of LEDS

- In motor vehicles and bicycle lights.
- In traffic light Indicators, signs and signals.
- In data displaying boards.
- In medical applications and toys.
- Non visual applications.
- In light bulbs and many more.
- Remote controls.

Conclusion

When looking at the long life spans and energy first choice when purchasing new bulbs for an area. As research continues, LEDs continue to improve and be used in new applications. With this new use for applications, there has been a major shift towards LEDs as a way to light everything from holiday lights to traffic signals. Due to the construction of LEDs, their ability to be efficient, durable, versatile, and longer lasting gives these bulbs a competitive edge when compared to the competition.

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Chapter III

Introduction to Silvaco TCAD and Simulation Steps

III.1 Introduction to the Simulation Program

III.1.1 Silvaco TCAD

Silvaco TCAD can be applied to a breadth and depth of applications useful in the development of semiconductor technologies. TCAD has been proven to be a powerful tool to provide in-depth understanding of device fabrication and operation. When applied by engineers to their Semiconductor R&D needs, TCAD can provide insights difficult or even impossible to achieve empirically. TCAD can help enhance device performance, increase yield and reduce time to market.

Figure III.1: SILVACO LOGO.

III.1.2 ATLAS

Atlas is a physically-based two and three dimensional device simulator. It predicts the electrical behavior of specified semiconductor structures and provides insight into the internal physical mechanisms associated with device operation.

Atlas can be used standalone or as a core tool in Silvaco’s Virtual Wafer Fab simulation environment. In the sequence of predicting the impact of process variables on circuit performance, device simulation fits between process simulation and SPICE model extraction.

Atlas is best used with the VWF Interactive Tools. These include DeckBuild, TonyPlot, DevEdit, MaskViews, and Optimizer. DeckBuild provides an interactive run time environment. TonyPlot supplies scientific visualization capabilities. DevEdit is an interactive tool for structure and mesh specification and refinement. MaskViews is an IC Layout Editor. The Optimizer supports black box optimization across multiple simulators.

Atlas, however, is often used with the Athena process simulator. Athena predicts the physical structures that result from processing steps. The resulting physical structures are used as input by Atlas, which then predicts the electrical characteristics associated with specified bias conditions. The combination of Athena and Atlas makes it possible to determine the impact of process parameters on device characteristics.

The electrical characteristics predicted by Atlas can be used as input by the Utmost device characterization and SPICE modeling software. Compact models based on simulated device characteristics can then be supplied to circuit designers for preliminary circuit design. Combining Athena, Atlas, Utmost, and SmartSpice makes it possible to predict the impact of process parameters on circuit characteristics.

Atlas can also be used as one of the simulators within the VWF Automation Tools. VWF makes it convenient to perform highly automated simulation-based experimentation. VWF is used in a way that reflects experimental research and development procedures using split lots. It therefore links simulation very closely to technology development, resulting in significantly increased benefits from simulation use.

III.1.2.1 Atlas Inputs and Outputs

Most Atlas simulations use two input files. The first input file is a text file that contains commands for Atlas to execute. The second input file is a structure file that defines the structure that will be simulated.

Atlas produces three types of output files. The first type of output file is the run-time output, which gives you the progress and the error and warning messages as the simulation proceeds. The second type of output file is the log file, which stores all terminal voltages and currents from the device analysis. The third type of output file is the solution file, which stores 2D and 3D data relating to the values of solution variables within the device at a given bias point.

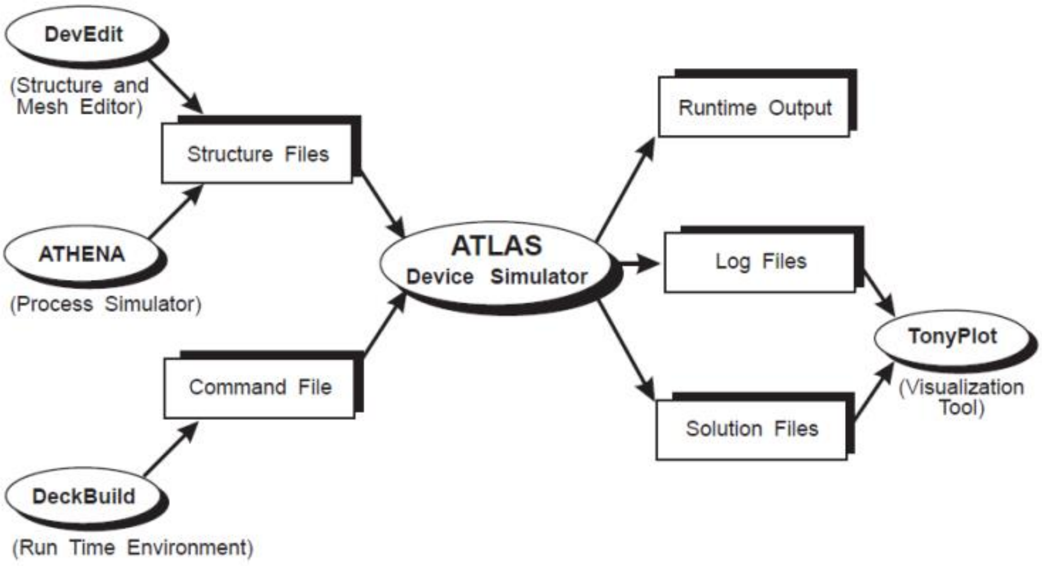
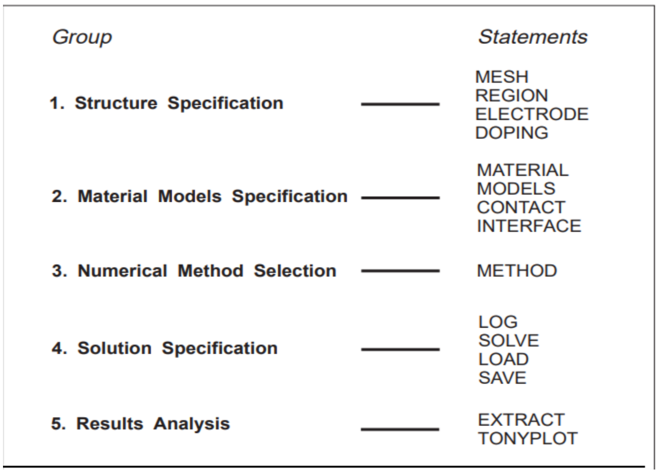


Figure III.2: Atlas Inputs and Outputs.

III.1.2.2 The Order of Atlas Commands

The order in which statements occur in an Atlas input file is important. There are five groups of statements that must occur in the correct order (see Figure below). Otherwise, an error message will appear, which may cause incorrect operation or termination of the program. For example, if the material parameters or models are set in the wrong order, then they may not be used in the calculations.

The order of statements within the mesh definition, structural definition, and solution groups is also important. Otherwise, it may also cause incorrect operation or termination of the program.



Group	*Statements*
1. Structure Specification	MESH REGION ELECTRODE DOPING
2. Material Models Specification	MATERIAL MODELS CONTACT INTERFACE
3. Numerical Method Selection	METHOD
4. Solution Specification	LOG SOLVE LOAD SAVE
5. Results Analysis	EXTRACT TONYPLOT

Figure III.3: Atlas Command Groups with the Primary Statements in each Group.

III.1.2.3 Accounting for quantum effects

In order to determine the bound energy states of quantum wells we introduce the parabolic quantum well model. Solving the Schrödinger equation gives a quantum description of the bound energy states in the quantum well. The effective masses and band parameters then derive from the 3-band k p model for constrained Wurtzite-type materials, initially developed by Chuang [01] and Chang [02], and incremented in the simulation code by the command wz.kp.

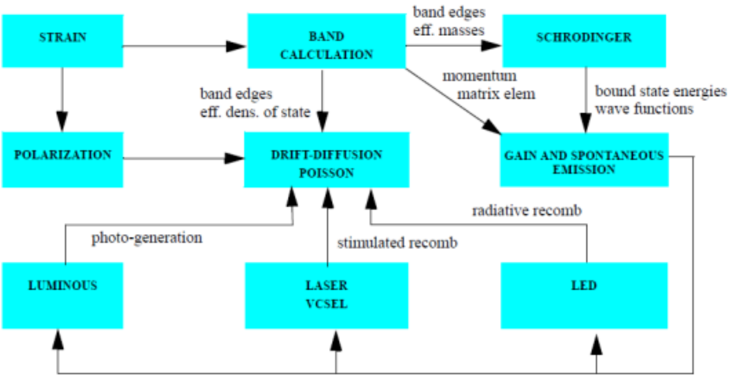


Figure III.4: Principle of simulation of optoelectronic devices in ATLAS.

III.2 Parameters of the Simulation

The simulation has been made with the environment of TCAD SILVACO using Atlas module. With the ability to predict the electrical characteristics of most semiconductors. In addition to external electrical properties, the software gives information about the internal distributions of variables such as lines of current, electric field and potentials. This is achievable by numerically solving the Poisson equation together with the continuity equations of electrons and holes at a finite number of points forming the structure mesh defined by are defined. The electroluminescent diode (LED) involves an array of thin semiconductor layers of GaN(n)/In$_x$Ga$_{1-x}$N(i)/GaN(i)/AlGaN(p)/GaN(p) simulate by TCAD Silvaco-Atlas. The complete device structure is schematically shown in Figure 3.6. In the present study the GaN layer (n-type) in the top, All wells are of InGaN(i), barriers are in GaN layer, electron blocking layer (EBL) is in AlGaN(p-type) and in the bottom the GaN(p-type).

All optical parameters used have been extracted from earlier reports [03] .During simulation by atlas TCAD, the physical models have been kept unchanged. The physical parameters for each layer are presented in Table III.1.

Table III.1: Used material Parameters in the simulation.

Parameters	**Value**		
Material	GaN	InGaN(i)	AlGaN(p)
Donor concentration Nd (cm^{-3})	5×10^{18}	–	–
Concentration of acceptors Na (cm^{-3})	1×10^{19}	–	1×10^{19}
Concentration of intrinsic carriers N_i	2×10^{16}	2×10^{16}	–
Electrons Mobility µn ($cm^2.V^{-1}.s^1$)	400	200	250
Hole mobility µp ($cm^2.V^{-1}.s^1$)	10	10	5
Electronic affinity χ (eV)	4.4	4.98	4.26
Band gap (at 300 K) E_g (eV)	3.42	2.6	3.62
Electron lifetime τn (s)	2×10^{-7}	2×10^{-7}	2×10^{-7}
Hole lifetime τp (s)	2×10^{-7}	2×10^{-7}	2×10^{-7}
Auger recombination coefficient Cn and Cp(cm−6.s−1)	2.4×10^{-30}	2.4×10^{-30}	2.4×10^{-30}

Table III.2: Models used in the simulation.

Parameters	**Model**
The energy bands	Model k.p
Recombination SRH	Model SRH
Recombination Auger	Model Auger
Recombination radiative	Model wz.kp
The mobility of electrons and holes	Mobility constants
The polarization field at the interfaces	Model Polarization, calc.strain and polar.scale
Ionization of carriers	Model incomplete

III.3 Internal electric field

Figure below represents the case of an InGaN well of thickness t_W surrounded by GaN barriers of thickness t_B. The energy levels of the excited states of the conduction and valence band as well as the gaps are represented there. In this case, the surface charge density σ.

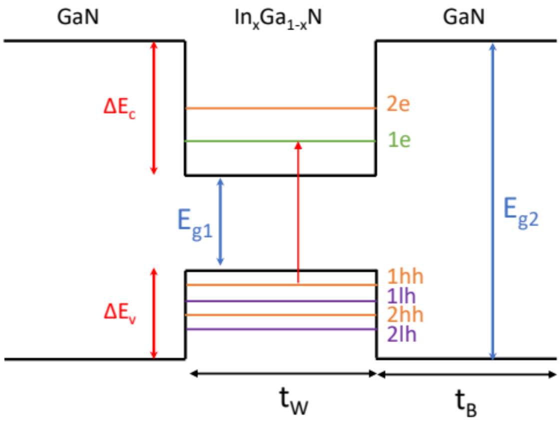


Figure III.5: Diagram of a GaN/InGaN quantum well.

III.4 Structure of the simulated LED

The objective of this chapter is to simulate the operation of a standard LED emitting in the blue whose architecture is illustrated in figure III.3. It is a rectangular LED with a section equal to 200 µm × 200 µm. The structure and geometric parameters of the LED are based on those mentioned in the literature, for example the LEDs simulated by Piprek et al.

This LED structure has (from top to bottom in Figure III.6):

— An n-doped GaN part (denoted "GaN-n") 3 µm thickness.

— An active zone composed of 6 quantum wells of InGaN at 16% indium 3 nm thickness separated by unintentionally doped 15 nm thick GaN barriers.

— An electron blocking layer (EBL) in AlGaN with 15% aluminum, 45 nm thickness.

— A p-doped GaN part (denoted "GaN-p") 200 nm thickness.

For each of the parts of this LED, the material parameters are summarized in Table III.1.

In order to take into account the physical mechanisms present in the LEDs, the models cited in Table III.2 are activated during the simulations. For the complete specificities of each model, the reader is invited to consult the ATLAS/SILVACO user manual.

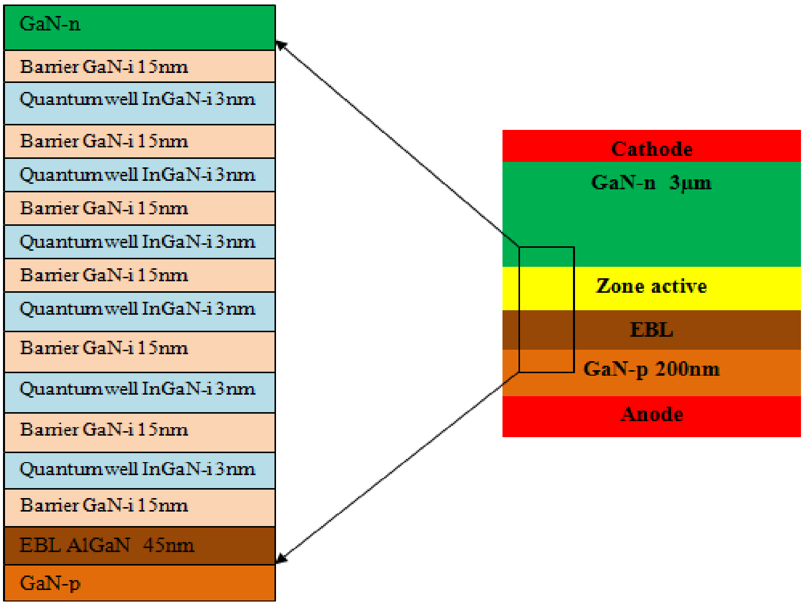


Figure III.6: Diagram of a standard LED based on III-N semiconductors.

III.5 Simulation steps

III.5.1 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.

The mesh used for this study is two-dimensional. Therefore, only x and y parameters are defined. The mesh is a series of horizontal and vertical lines and spacing between them. From Figure III.9, the mesh statements are specified.

The general format to define the mesh is:

X.MESH LOCATION=<VALUE> SPACING=<VALUE>

Y.MESH LOCATION=<VALUE> SPACING=<VALUE>

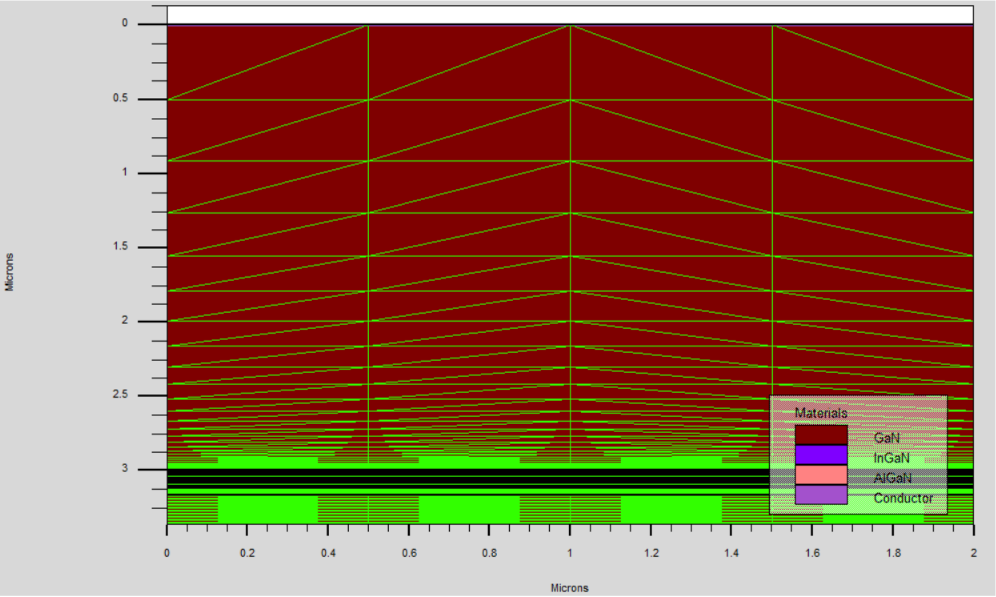
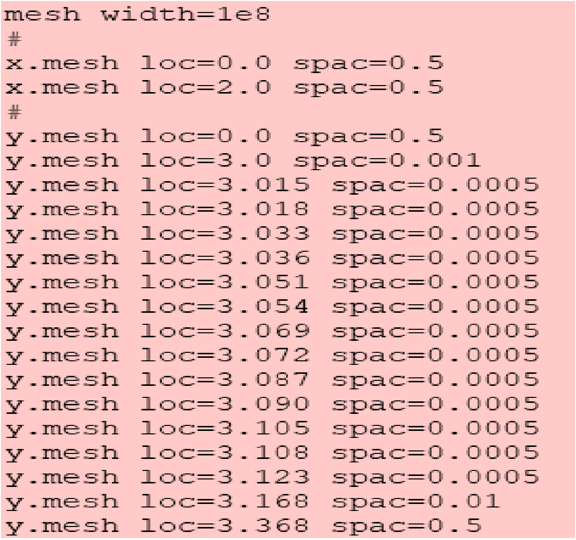


Figure III.9: 6 multiple quantum well LED mesh.

In our work, the x.mesh starting at 0 microns to 2.0 microns has spacing of 0.5 microns. That means it is relatively coarse. The y.mesh is similarly defined; the y.mesh started at 0 microns and ends in 3.368 microns as we can see in the Figure III.10.



```
mesh width=1e8
#
x.mesh loc=0.0 spac=0.5
x.mesh loc=2.0 spac=0.5
#
y.mesh loc=0.0 spac=0.5
y.mesh loc=3.0 spac=0.001
y.mesh loc=3.015 spac=0.0005
y.mesh loc=3.018 spac=0.0005
y.mesh loc=3.033 spac=0.0005
y.mesh loc=3.036 spac=0.0005
y.mesh loc=3.051 spac=0.0005
y.mesh loc=3.054 spac=0.0005
y.mesh loc=3.069 spac=0.0005
y.mesh loc=3.072 spac=0.0005
y.mesh loc=3.087 spac=0.0005
y.mesh loc=3.090 spac=0.0005
y.mesh loc=3.105 spac=0.0005
y.mesh loc=3.108 spac=0.0005
y.mesh loc=3.123 spac=0.0005
y.mesh loc=3.168 spac=0.01
y.mesh loc=3.368 spac=0.5
```

Figure III.10: mesh defined in SILVACO .

The spacing has different values in y.mesh . The mesh is coarser at y.mesh location of 0 to 3 microns cause it’s the n.doped GAN.

The y.mesh is a lot smaller from 3.015 to 3.123 with a spacing of 0.0005 microns because it’s the active zone and we need to study the wells and barriers.

The mesh is coarser at y.mesh location of 3.168 to 3.368 microns cause it’s the EBL and p.doped GAN.

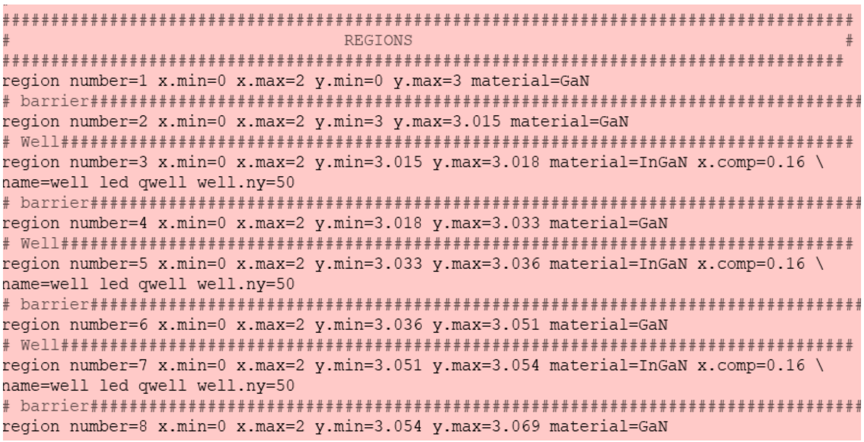
The right choices of meshing play important roles in the simulation accuracy. The simulation mesh represents the points (nodes) of the structure at which the model equations are solved. Thus, the right specifications and the number of nodes in the grid are necessary for simulation time saving and accuracy. A finer mesh should be available especially in the simulation structure critical areas, where ion implantation occurs or where wells existed. In the present structure, the mesh is made non-uniform, but fine only into critical regions. If the mesh is fine in all structure, the simulation time becomes too long due to time loss in the non-critical region.

III.5.2 Region

After defining the mesh, it is necessary to define the regions. The format to define the regions is as follows:

REGION number=<integer><material_type> / <position parameters>

From Figure 3.11, the code that defines the regions is identified. The limits of each region are explicitly identified in the x and y axis. The regions must then be given a material.



```
#######################################################################################
#                                  REGIONS                                            #
######################################################################################
region number=1 x.min=0 x.max=2 y.min=0 y.max=3 material=GaN
# barrier###############################################################################
region number=2 x.min=0 x.max=2 y.min=3 y.max=3.015 material=GaN
# Well#################################################################################
region number=3 x.min=0 x.max=2 y.min=3.015 y.max=3.018 material=InGaN x.comp=0.16 \
name=well led qwell well.ny=50
# barrier###############################################################################
region number=4 x.min=0 x.max=2 y.min=3.018 y.max=3.033 material=GaN
# Well#################################################################################
region number=5 x.min=0 x.max=2 y.min=3.033 y.max=3.036 material=InGaN x.comp=0.16 \
name=well led qwell well.ny=50
# barrier###############################################################################
region number=6 x.min=0 x.max=2 y.min=3.036 y.max=3.051 material=GaN
# Well#################################################################################
region number=7 x.min=0 x.max=2 y.min=3.051 y.max=3.054 material=InGaN x.comp=0.16 \
name=well led qwell well.ny=50
# barrier###############################################################################
region number=8 x.min=0 x.max=2 y.min=3.054 y.max=3.069 material=GaN
```

Figure III.11: The region defines in SILVACO.

From Figure III.12, the code defines the material for each region. Note that the color coding identifies the material. The regions have vertical and horizontal lines to mark their boundaries.

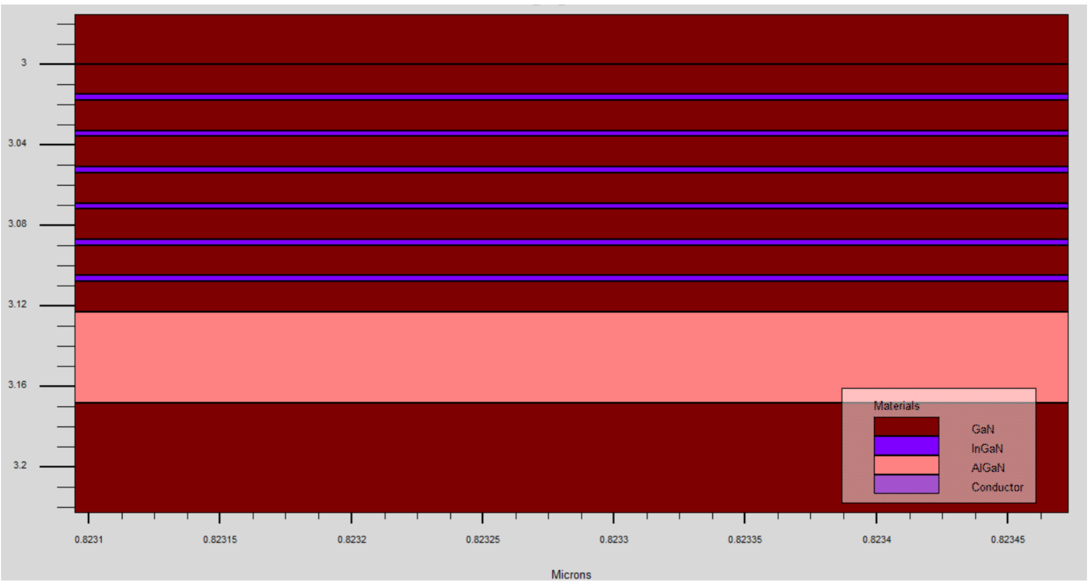


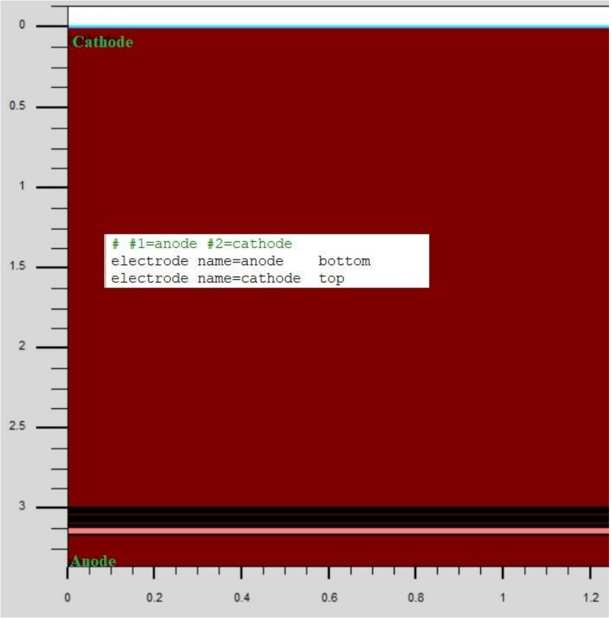
Figure III.12: Materials used in this simulation.

III.5.3Electrodes

The next structure specification corresponds to electrodes. Typically, in this simulation the only electrodes defined are the anode and the cathode. The format to define electrodes is as follows:

ELECTRODE NAME=<electrode name><position_parameters>

From Figure III.13, the electrode statements are defined for the anode and the cathode. The anode is defined at the bottom and the cathode is defined at the top.



```
# #1=anode #2=cathode
electrode name=anode    bottom
electrode name=cathode  top
```

Figure III.13: the electrode in the mesh and structure.

III.5.4 Doping

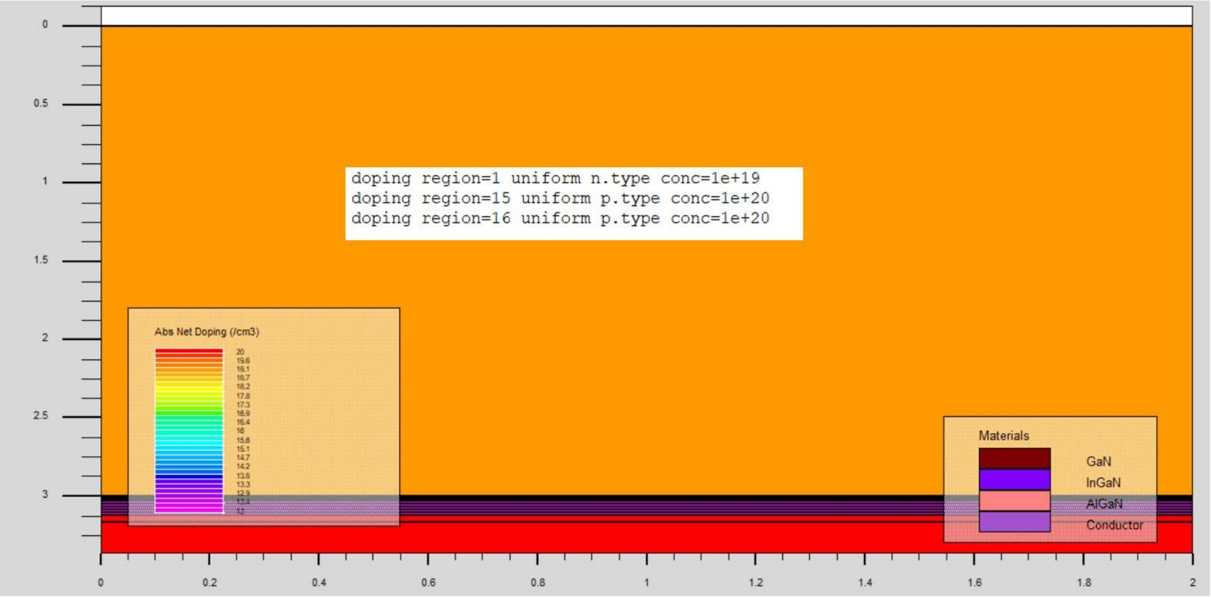
The last aspect of structure specification that needs to be defined is doping. The format of the

Atlas statement is as follows:

DOPING <distribution type> <dopant_type> < concentration value>

From Figure 3.14, shows the doping types and the doping levels are defined. Doping can be n-type or p-type. The distribution type is uniform.

The doping happen only 3 region the region 1 in GaN with n-type with p-type with concentration of 1e+19 and region 15 in AlGaN with p type with p-type with concentration of 1e+20 and region 16 with p-type with concentration of 1e+20 .



```
doping region=1 uniform n.type conc=1e+19
doping region=15 uniform p.type conc=1e+20
doping region=16 uniform p.type conc=1e+20
```

Figure III.14: Doping in the mesh and structure.

III.5.5 Materials and Model Specification

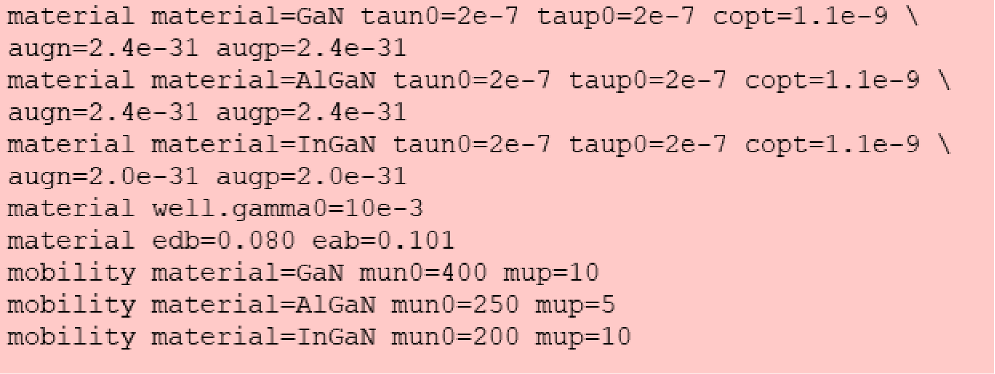
After the structure specification, the materials model specification is next.

III.5.5.1 Materials

The format for the material statement is as follows:

MATERIAL <localization><material_definition>

Below in the Figure 3.15 is the material used in this simulation



```
material material=GaN taun0=2e-7 taup0=2e-7 copt=1.1e-9 \
augn=2.4e-31 augp=2.4e-31
material material=AlGaN taun0=2e-7 taup0=2e-7 copt=1.1e-9 \
augn=2.4e-31 augp=2.4e-31
material material=InGaN taun0=2e-7 taup0=2e-7 copt=1.1e-9 \
augn=2.0e-31 augp=2.0e-31
material well.gamma0=10e-3
material edb=0.080 eab=0.101
mobility material=GaN mun0=400 mup=10
mobility material=AlGaN mun0=250 mup=5
mobility material=InGaN mun0=200 mup=10
```

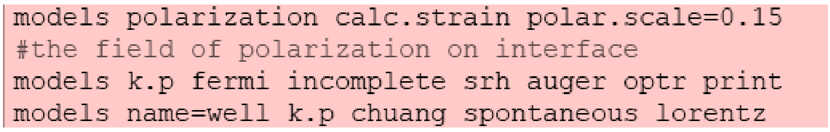
Figure III.15: materials used in this simulation.

III.5.5.2 Models

The physical models fall into five categories: mobility, recombination, carrier statistics, impact ionization, and tunneling. The syntax of the model statement is as follows:

MODELS <model flag><general parameter> / <model dependent parameters>

The choice of model depends on the materials chosen for simulation. The figure 3.16 shows several models used in this simulation.



```
models polarization calc.strain polar.scale=0.15
#the field of polarization on interface
models k.p fermi incomplete srh auger optr print
models name=well k.p chuang spontaneous lorentz
```

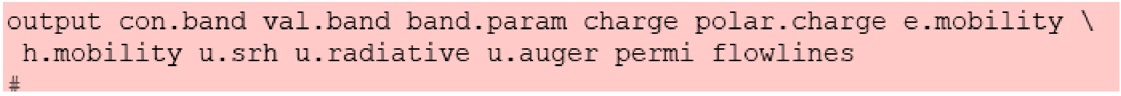
Figure III.16: used models.

III.5.6 Methods and Solution

III.5.6.1 Output flags and Methods

We use different flags and methods in this simulation to gain various results to help us study the LED and its characteristic.

In the Figure 3.17 we see the Output flags and Methods used in this simulation.



```
output con.band val.band band.param charge polar.charge e.mobility \
 h.mobility u.srh u.radiative u.auger permi flowlines
#
```

Figure III.17: Output flags and Methods.

III.5.6.2 Numerical Method Selection and Solution Specification

After the materials model specification, the numerical method selection must be specified. There are various numerical methods to calculate solutions to semiconductor device problems. There are three types of solution techniques used in Silvaco Atlas:

- Decoupled (GUMMEL)
- Fully coupled (NEWTON)
- BLOCK

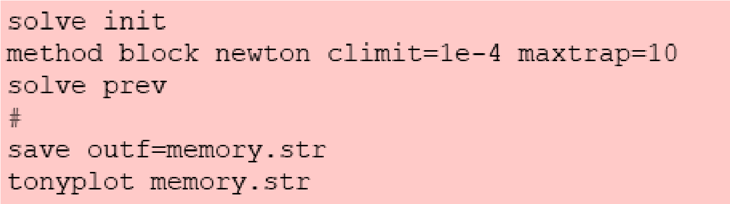
The GUMMEL method will solve for each unknown in turn keeping the other variables constant, repeating the process until a stable solution is achieved.

The NEWTON method solves the total system of unknowns together.

The BLOCK methods will solve some equations fully coupled while others are de-coupled.

In This simulation we used the BLOCK NEWTON method.

After completing the numerical method selection, the solution specification is next. Solution specification is broken down into log, solve, load, and save statements as we can see in the figure 3.18.



```
solve init
method block newton climit=1e-4 maxtrap=10
solve prev
#
save outf=memory.str
tonyplot memory.str
```

Figure III.18: Numerical Method Selection.

III.5.6.3 Solution Specification

After completing the numerical method selection, the solution specification is next. Solution specification is broken down into log, solve, load, and save statements.

Log files (.log) store the terminal characteristics calculated by Atlas. The following shows an example of the LOG statement.

LOG OUTFILE=myoutputfile.log

The SOLVE statement follows the LOG statement. SOLVE performs a solution for one or more bias points. The following is an example of the SOLVE statement.

Solve vstep=0.5 vfinal=2.5 name=anode

The LOAD statement enters previous solutions from files as initial guess to other bias points.

The SAVE statement enters all node point information into an output file.

The following are examples of LOAD and SAVE statements.

Save outf=led_test_2.5.str

The figure Figure 3.19 shows the solution Specification in this simulation

```
log outf=led_test.log
solve vstep=0.5 vfinal=2.5 name=anode
save outf=led_test_2.5.str spectrum=2.5.log
save spectrum=led_test_2.5.spc lmin=0.35 lmax=0.55 nsamp=200
solve vstep=0.5 vfinal=3.0 name=anode
save outf=led_test_3.str spectrum=3.log
save spectrum= led_test_3.spc lmin=0.35 lmax=0.55 nsamp=200
solve vstep=0.5 vfinal=3.5 name=anode
save outf=led_test_3.5.str spectrum=3.5.log
save spectrum= led_test_3.5.spc lmin=0.35 lmax=0.55 nsamp=200
solve vstep=0.5 vfinal=4.0 name=anode
save outf=led_test_4.str spectrum=4.log
save spectrum= led_test_6.spc lmin=0.35 lmax=0.55 nsamp=200
solve vstep=0.5 vfinal=6 name=anode
save outf=led_test_6.str spectrum=6.log
#I-V Curve
tonyplot led_test.log -set ledex02_0.set
# I-L Curve
tonyplot led_test.log -set ledex02_1.set
# EL Spectrum
tonyplot led_test_3.5.spc -set ledex02_2.set
```

Figure III.19: Solution Specification.

Once a solution has been found for a semiconductor device problem, the information can be displayed graphically with TonyPlot. Additionally, device parameters can be extracted as well.

Chapter IV
Results and discussions

This work is to study characteristic of LED based of InGaN quantum wells with different simulations to understand how it works in terms of which light color we can reach or the power of the output light ...etc.

IV.1 Study of 6 quantum wells

First of all, basic 6 MQW LED model is established based on the nature of GaN and InGaN, and all of the simulated results are on the basis of the drift-diffusion equations.

The proposed structure of InGaN/GaN MQW LED is shown in Figure IV.1; it was simulated using ATLAS in SILVACO TCAD device simulation.

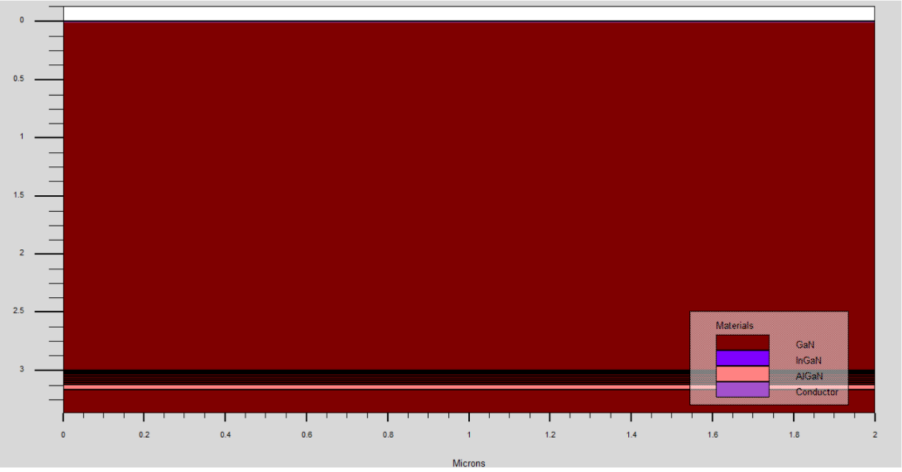


Figure IV.1: Structure of the 6 quantum well LED.

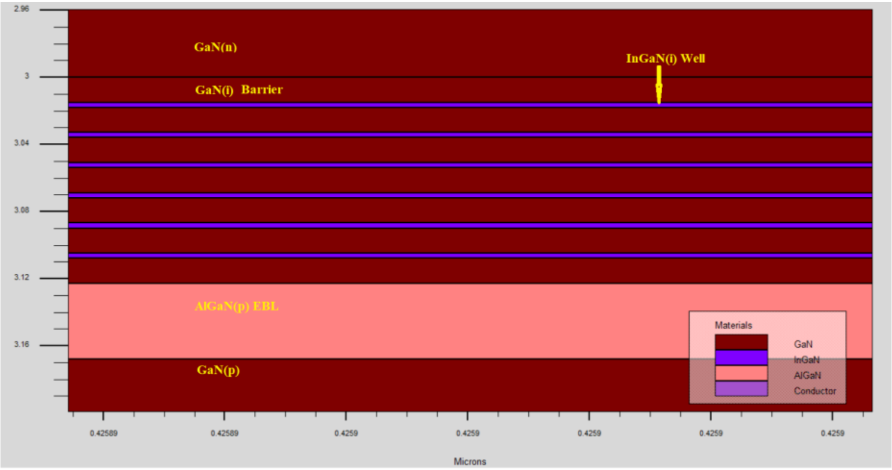


Figure IV.2: closer look at Structure of the multiple quantum well LED.

IV.1.1 Doping

In the figure IV.3 it shows the doping concentration.

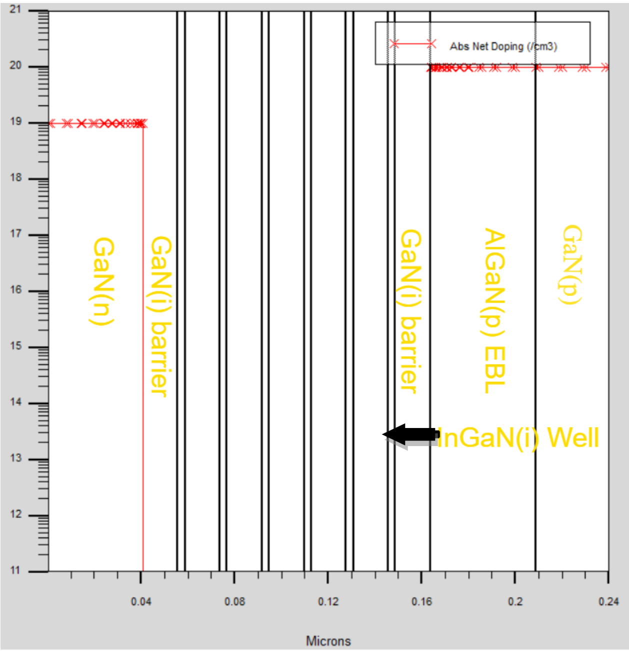


Figure IV.3: Doping concentration in the LED.

As we can see the doping concentration in the GaN(n) layer is 10^{19}cm^{-3} and in GaN(p) layer and EBL layer is 10^{20}cm^{-3} but in the wells and barriers the concentration is 0 because the semiconductors are Intrinsic.

IV.1.2 Band diagram of MQW:

The band diagram of the LED structure is shown in Figure below It shows five quantum wells in the band structure. It is evident from the band structure that.

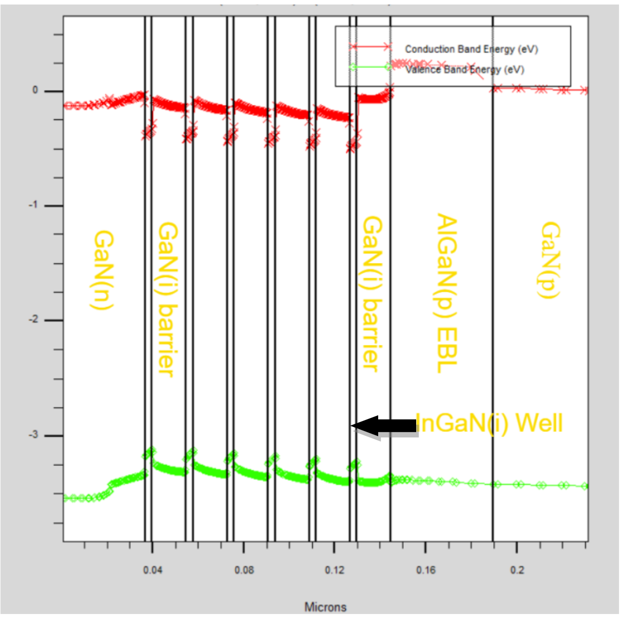


Figure IV.3: Energy band diagram of MQW active region.

The energy in the band diagram (EC and EV) is different between the barrier (GaN) and the well (InGaN) due to the difference in the EG GaN is 3.42 and InGaN is 2.6.

IV.1.3 Recombination rate:

In the figure 4.4 we see the different recombination rate in the structure (Auger, Radiative and SRH).

The recombination happen only the quantum wells and the barriers function to keep the electrons in the well for better recombination rate.

The SRH recombination is so low compared to auger and radiative recombination.

This due to the intrinsic type of the quantum well and barrier, the thinner thickness of wells the the greater thickness of barriers in which it avoids the passage of charge carriers by tunnel effect , and we that the recombination rate is different between the wells, this due to the flow and the mobility of charges from the two sides GaN(n)and GaN(p), Moreover the election blocking layer EBL which stops the passage of holes and eelctons to the GaN(p) limit side.

The radiative recombination reaches in the 6 well $7.8\times10^{28}\text{cm}^{-3}$/s but the auger recombination reaches only $1\times10^{28}\text{cm}^{-3}$/s.

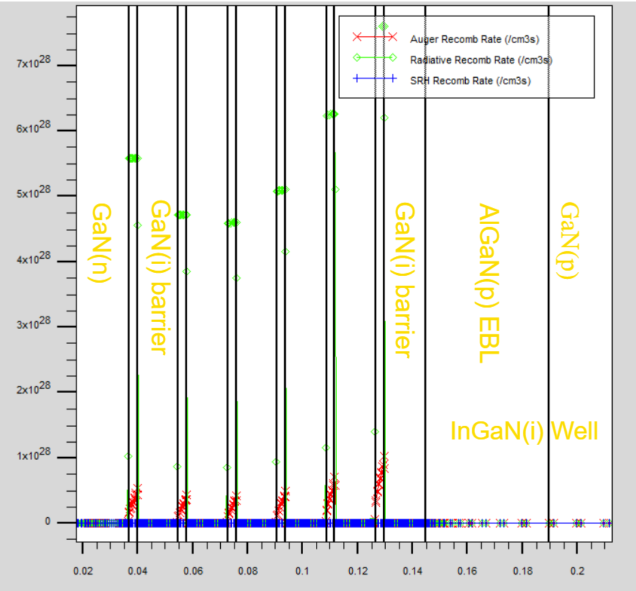


Figure IV.4: Auger, SRH and Radiative recombination in the structure.

In the figure IV.5 we have the graph of the Radiative recombination in the variation of the voltage in the Anode.

From 0V to 3V the Radiative recombination rate is 0 and from the 3V to 6V the Radiative recombination rate start to increase significantly with the voltage increase and its reach its highest point in the $1.8\times10^{24}cm^{-3}/s$.

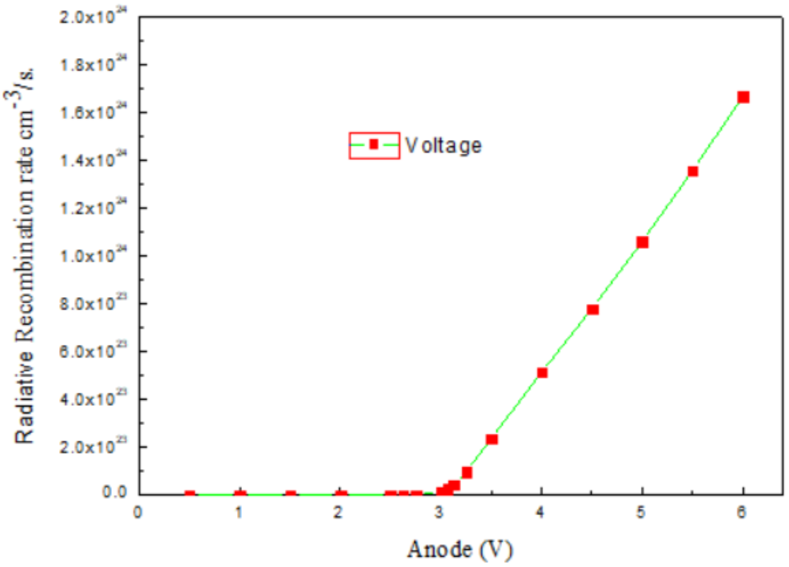


Figure IV.5: Radiative recombination in the structure.

IV.1.4 Luminous Power total

The obtained results make the proposed structure very useful for future technology. Accordingly, the variation of luminous intensity versus the anode voltage is shown in Figure 4.6.It is clear that as the anode voltage increases, more the luminous is increased and reaches its maximum value.

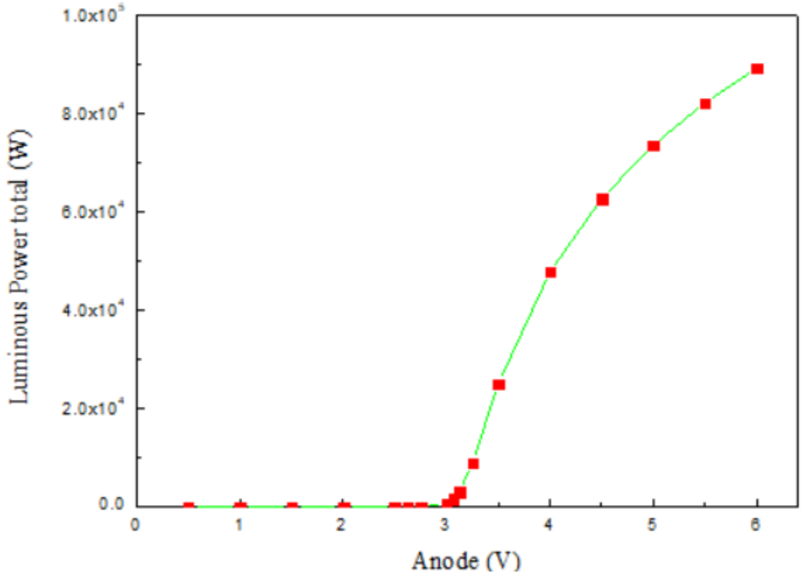


Figure IV.6: Luminous Power total in the structure.

IV.1.5 I-V characteristic

By implementing the simulation parameters mentioned in previous Table, the I-V characteristic of the analyzed structure can be given in Figure 4.7. From the figure, it can be seen that the structure provides high anode current at value 6V of anode voltage. Therefore, the threshold is about 3V which is less than other standard structures.

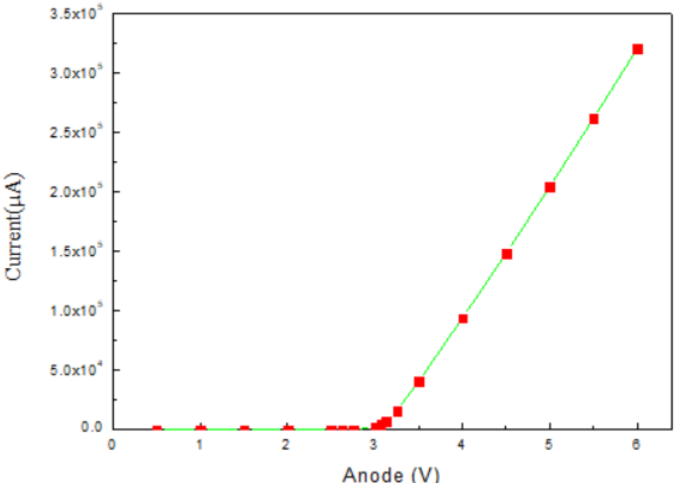


Figure IV.7: I-V characteristics of MQW LED structure.

IV.1.6 Spectrum of Emitted Light

The radiation emitted by a light-emitting diode is not monochromatic but it has a spectral distribution centered on the most probable wavelength fixed by the width Eg of the forbidden band. In the Figure IV.8 the wavelength is almost between 0.39 and 0.44 so the color of this led is violet.

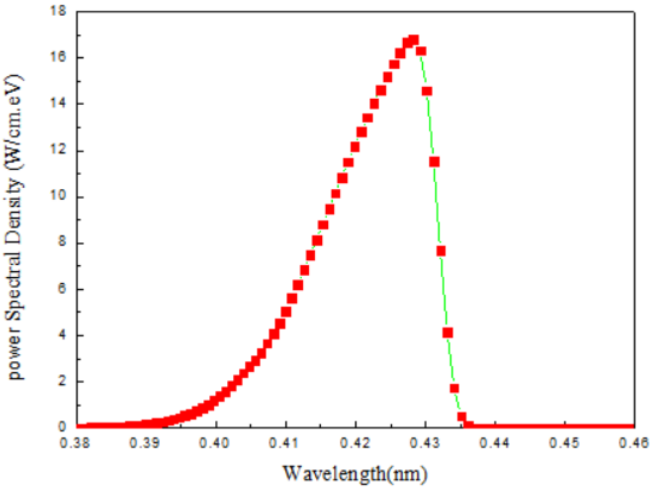


Figure IV.8: I Spectrum of Emitted Light.

IV.2 Effect of different number of quantum wells

In the second study we did we tried to see the difference between single well and multi-quantum wells to what change in the characteristic we will have as a results.

IV.2.1 diagram of different quantum wells

The figure IV.9 represents the structure of the active zone to different number of quantum wells from 1 QW to 6 QW.

The thickness increase from 1 QW to 6 QW.

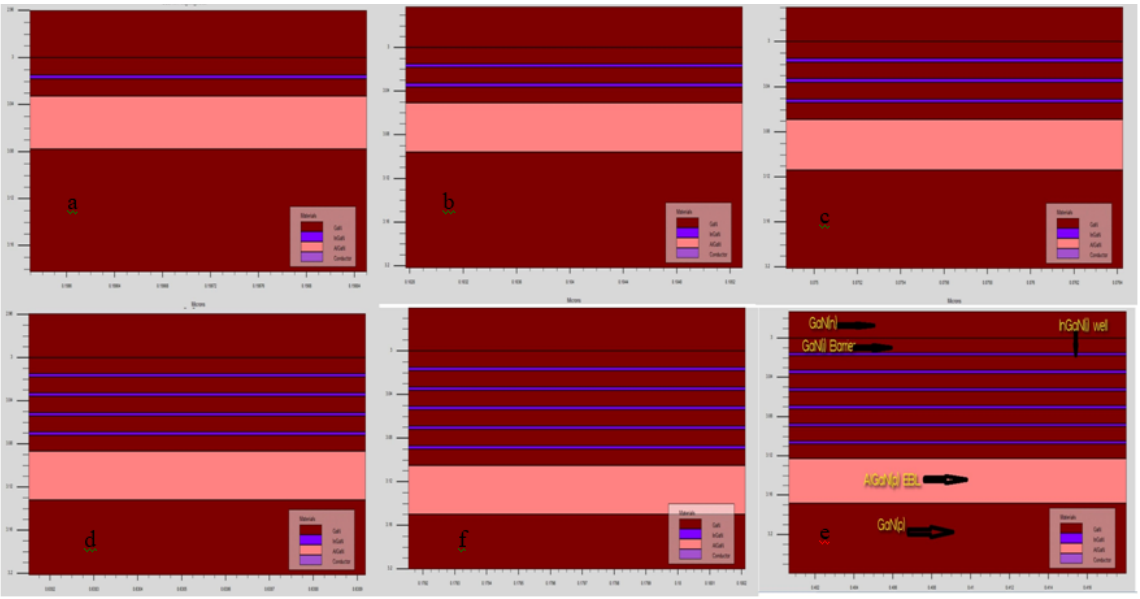


Figure IV.9: I Spectrum of Emitted Light.

Now we are going to study the difference in the characteristic of multi-wells.

IV.2.2 Recombination rate

In the figure IV.10, we see the different radiative recombination rate in different quantum wells.

As we can see in the figure IV.10 when we add a new QW, the Radiative recombination rate increase in the first 3 QW but in 4,5 and 6 QW they are almost the same value .this increasing due to the confine of the charge carriers in wells and the thinner thickness of quantum well, which means that we increase the probability of the recombination rate in this active zone, moreover the number of well has a positive impact in which it increase the radiative recombination in wells. The total recombination become the sum of all individual recombination exists in each quantum well.

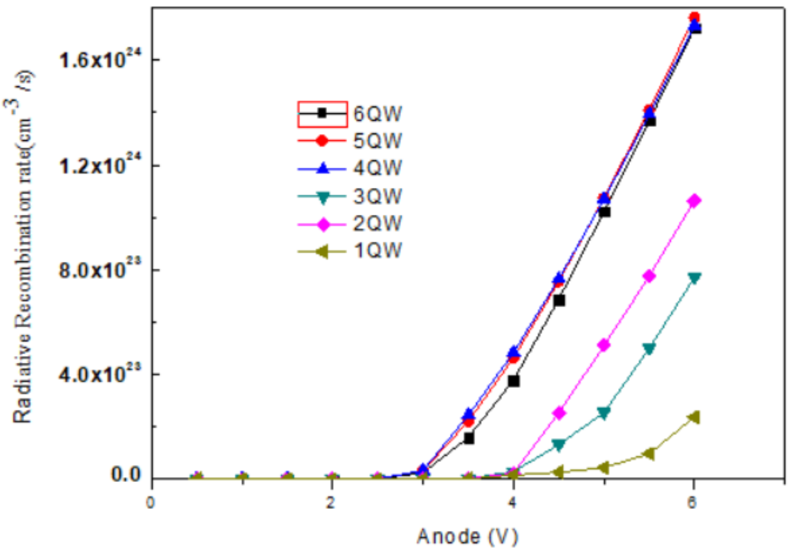


Figure IV.10: Radiative recombination rate in different QW.

IV.2.3 Luminous Power total

The variation of luminous intensity versus the anode voltage is shown in Figure IV.6 of different QW.

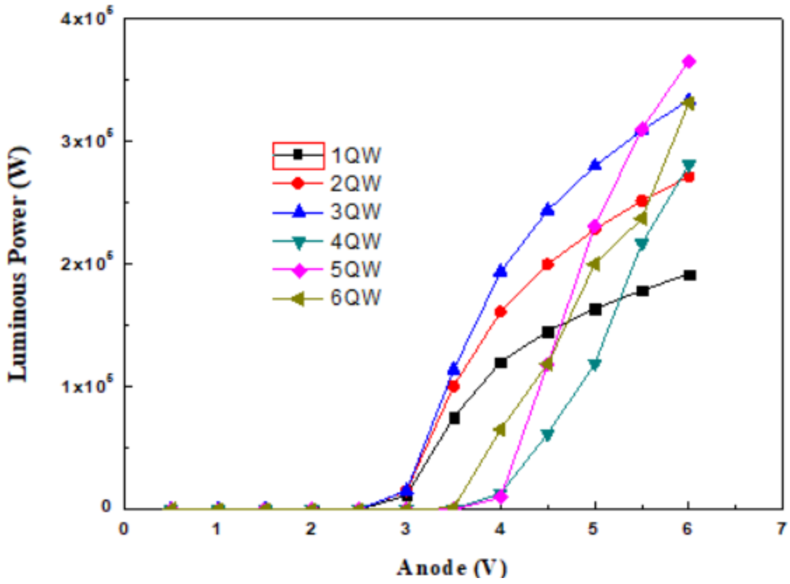


Figure IV.11: Luminous Power total in different QW.

From figure IV.11 every QW has different Luminous Power and it increases with adding new QW in the structure .this due to the increasing of radiative recombination phenomena in the active zone caused the confinement of the charge carriers in the quantum wells.

IV.2.4 I-V characteristic

The I-V characteristic of current vs voltage of different quantum wells. If we look at the figure IV.12 we can see 1 to 3 QW have almost the same value and when we go to 4 QW its to decrease significantly till it reaches the lowest point in 6 QW.

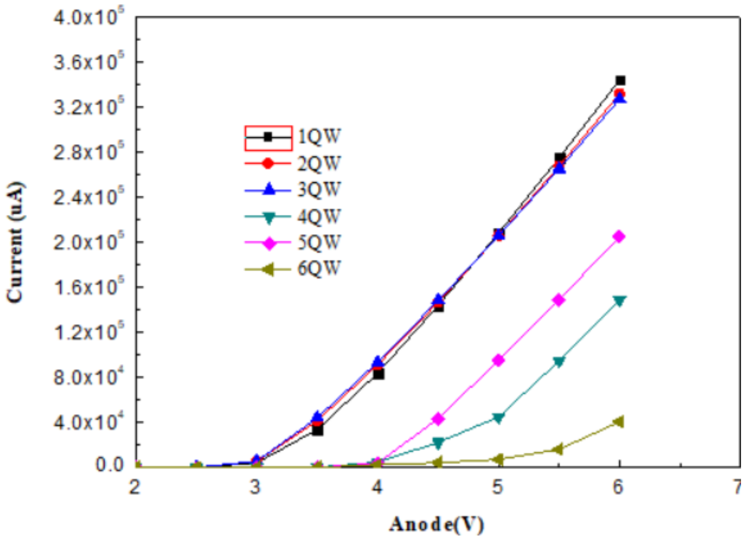


Figure IV.12: I-V characteristic of different quantum wells

IV.2.5 Spectrum of Emitted Light

In the Figure 4.13 after we study the power Spectral Density vs the wavelength we find the power Spectral Density is different and decreases whenever we add a new QW and the wavelength is almost the same between 0.36 and 0.44 so it generate the violet color in this LEDs.

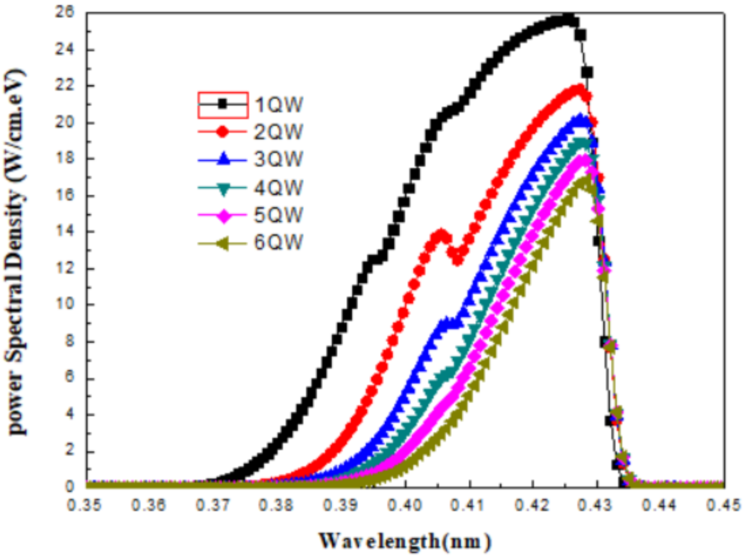


Figure IV.13: Power Spectral density vs Wavelength in different QW.

IV.3 Effect of different mole fractions (x) in 6 quantum wells

In this study we try to change the mole fractions in InGaN to see the effects in the LED characteristic.

We calculate the EG and the wavelength by using Vegard's Law as can see below in Table IV.1.

$$Eg(x) = (1-x)\times Eg(GaN)+x\times Eg(InN)-b\times x\times(1-x) \qquad (08)$$

$$h\upsilon = \frac{hc}{\lambda} = Eg \qquad (09)$$

Where b is the "bowing parameter" of the Eg(x) curve. The value of x for each InxGa1-xN sample was determined in the experimental work by x-ray diffraction measurement of the sample lattice parameters and application of Vegard's Law.

The evaluation here sets Eg(GaN) as 3.4eV and Eg(InN) 0.7eV respectively, and b as 1.00 eV (Nakamura 1994).

Corresponding Optical Wavelength is λ .and hc is 1.24.

Indium Content (x)	Energy Gap (eV)	Corresponding Optical Wavelength (nm)
0.02	3.3264	0.373
0.04	3.2536	0.381
0.08	3.1104	0.399
0.10	3.04	0.408
0.12	2.9704	0.418
0.16	2.8336	0.438
0.18	2.7664	0.448

Table IV.1: Eg and wavelength calculation.

After calculating EG and wavelength as we see the results in this table we can say the more we add mole fraction to the InGaN the less the EG and wavelength get more.

Also the wavelength of the x=0.02 is ultraviolet which is invisible to human eye and the others once are all visible violet.

IV.3.1 Recombination rate

In the figure IV.14 we see the different Radiative recombination rate in 6 quantum wells with different mole fractions.

As we can see in the figure IV.10 when x=0.02 the Radiative recombination rate have the highest value and when x=0.16 have the lowest value.

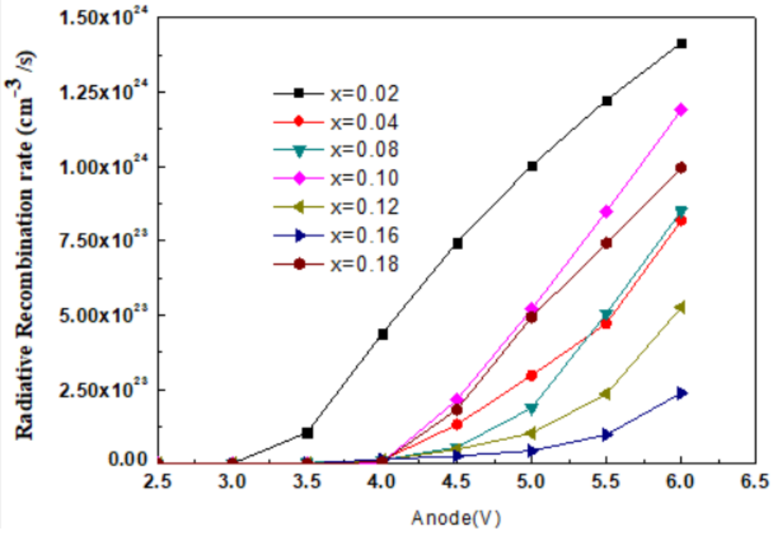


Figure IV.14: Radiative recombination rate vs voltage in 6QW with different mole fractions.

IV.3.2 Luminous Power total

The variation of luminous intensity versus the anode voltage is shown in Figure IV.6 of different QW.

as we can see in the figure IV.15 we change the value of mole fraction from 0.02 to 0.18 we found a various graphs and the one with the highest luminous power total is x=0.02 and the lowest is x=0.16.

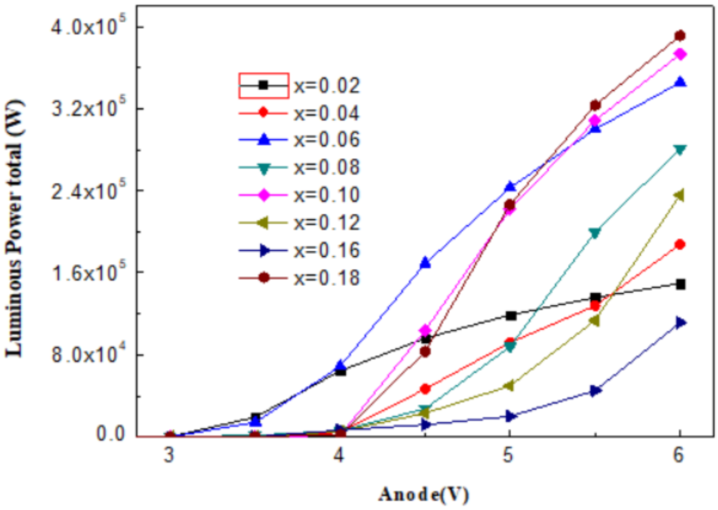


Figure IV.15: Luminous Power total in different mole fractions .

IV.3.3 I-V characteristic

If we look at the figure IV.16 we can see the LED with highest value is the x=0.02 and the lowest value is x=0.16 but the x=0.10 and x=0.18 have almost graph.

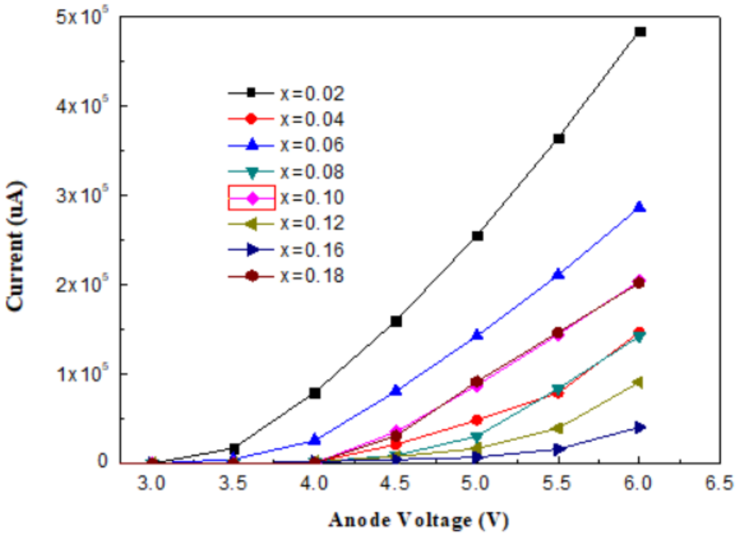


Figure IV.16: The I-V characteristic of different mole fraction.

IV.3.4 Spectrum of Emitted Light

In the Figure IV.17 after we study the power Spectral Density vs the wavelength we find the power Spectral Density is different and have random values when we change the mole fraction and the wavelength also different there are colors in the infrared light and Visible Light (violet).

x= 0.02, 0.04 are in the infrared light wavelength.

Others values are visible light and its color is violet.

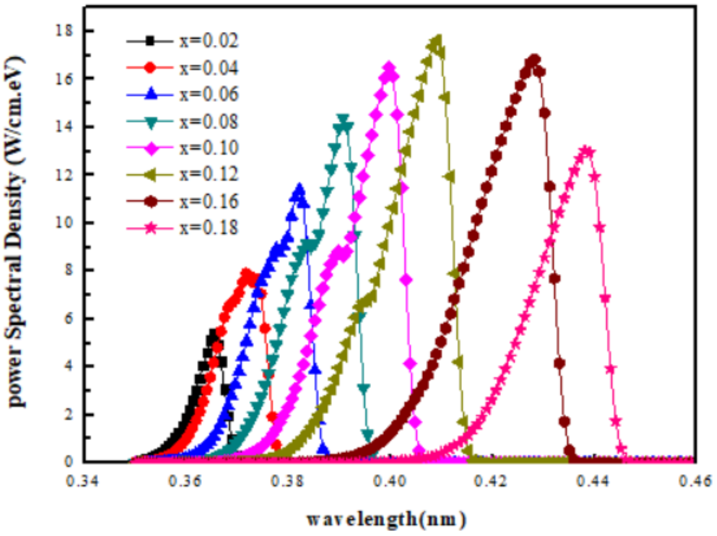


Figure IV.17: power Spectral Density vs Wavelength in different mole fractions.

Conclusion

In summary, we developed a MQW for practical application .In the first study we found the characteristics of 6 QW.

In the second study we changed the QW from 1 to 6 wells to see the effects in the characteristics and the results we observed the change happened in current , Recombination rate, Luminous Power total, Spectrum of Emitted Light, power Spectral Density but the wavelength stays the same which means changing the the number of wells won’t change the wavelength so the color will stay the same .

In the third study we changed the mole fraction for different values from 0.02 to 0.18 and we observed that it changes all the characteristics of the LED.

General Conclusion

LED lighting technology is quickly becoming the dominant source of lighting in the modern world. The numerous advantages that solid-state lighting technology possesses over conventional incandescent light bulbs or CFLs like much lower electrical power consumption, longer life, non-toxicity and higher durability are the major factors that are driving the growth of this industry. The ability to produce light having energy high up in the spectrum meant it could be used for a large variety of applications.

In this study we analyzed different characteristics: first we found the number of QW increased the recombination rate which affected the luminosity power to change to higher numbers, but the QW change decreased the current, the wavelength didn’t change at all.

In the second Study we analyzed the characteristics as the first one but we kept number of wells the same (6QW) and changed the mole fraction the result we found the change happened in all characteristics so this time even the wavelength changed.

So In conclusion we found the number of quantum wells and mole fraction play an important role in determining the optical and electrical characteristics of the InGaN/GaN MQWs.

Abstract

III-V nitride semiconductor materials are useful for light emitting device in short wavelength region due to their relatively wide band gap and high emission efficiency.

Different types and structures have been previously studied. In our work, multi quantum well (MQW) LED based on InGaN/GaN using Silvaco-Atlas software has been simulated and studied.

The performance of InGaN quantum well based Light Emitting Diodes (multi quantum wells); (LEDs) had been numerically investigated by Tcad-Silvaco. We simulated different characteristics in this study to see the effect it will make in terms of wavelength, I-V characteristic, Luminosity power and Radaitive Recombination rate.

Les matériaux semi-conducteurs à base de nitrure III-V sont utiles pour les dispositifs émetteurs de lumière dans la région des courtes longueurs d'onde en raison de leur bande interdite relativement large et de leur haute efficacité d'émission.

Différents types et structures ont été précédemment étudiés dans la littérature. Dans notre travail, une LED à puits quantiques multiples (MQW) basée sur InGaN/GaN utilisant le logiciel Silvaco-Atlas a été simulée et étudiée.

Les performances des diodes électroluminescentes (LED) à base de puits quantiques en InGaN (multi quantum wells) ont été étudiées numériquement par Tcad-Silvaco. Nous avons simulé différentes caractéristiques dans cette étude pour voir l'effet qu'elles auront en termes de longueur d'onde, de caractéristique I-V, de puissance lumineuse et de taux de recombinaison radaitive.

تعتبر مواد أشباه الموصلات من نيتريد III-V مفيدة لانبعاث الضوء في منطقة الطول الموجي القصير بسبب فجوة النطاق العريضة نسبيًا وكفاءة الانبعاث العالية.

تمت دراسة أنواع وتركيبات مختلفة مسبقًا. في عملنا ، تمت محاكاة ودراسة LED متعدد الآبار (MQW) بواسطة الثنائية InGaN / GaN باستخدام برنامج Silvaco-Atlas.

أداء الثنائيات الباعثة للضوء InGaN ذات الأساس الكمي (الآبار الكمومية المتعددة) ؛ تم دراسة و تحليل (LEDs) حسابيا بواسطة Tcad-Silvaco. قمنا بمحاكاة الخصائص المختلفة في هذه الدراسة لمعرفة التأثير الذي ستحدثه من حيث الطول الموجي وخاصية I-V وشدة الاضاءة ومعدل إعادة التركيب الإشعاعي.