DOPANTS CONCENTRATION EFFECT ON GALLIUM ARSENIDE AND GALLIUM NITRIDE-BASED HOMOJUNCTION LED EPI-LAYERS

BY

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ABSTRACT

This work reports the effect of doping on the energy-band structure of homojunction light-emitting diode (LED) epitaxial layers. The research correlates the resultant values of bandgap energy and its depletion region, which are then applied to the luminescence spectrum of the light-emitting diode. The energy-band structure is simulated by initializing the various materials' properties of Gallium Nitride (GaN), including Gallium Arsenide (GaAs), and solving the Poisson's equation derived from Boltzmann's Transport equation. The equation is solved by applying the finite difference method and using the Newton-Raphson method. Both materials are compared with different dopant concentrations in the range of 1×10^{18} cm^{-3} to 1×10^{21} cm^{-3}. Taking the Silicon properties as the controlled variable, the energy-band structure is validated with literature findings. The calculated band gap energy of GaAs shifts from 1.4273 eV to 1.4640 eV, and for GaN, from 3.3970 eV to 3.4148 eV. The bandgap energy increases with the proportion to the doping concentration increments. However, when obtaining the epitaxial layer's active 1-D spatial regions for GaAs and GaN, it reduces from (1.5700×10^{-1} µm – 7.5000×10^{-3} µm) and from (1.8450×10^{-1} µm – 8.5000×10^{-3} µm) x 1 μm^2 respectively. The findings show that doping concentration is saturated at a certain threshold, which provides a less significant impact on the semiconductor energy-band structure. Thus, the numerical system determines the LED output spectrum and the threshold values for bandgap energy. The analyzed bandgap thresholds are obtained as 1.440eV for GaAs and 3.403eV for GaN at dopants' concentrations of $2.951 \times 10^{19} cm^{-3}$ and $4.467 \times 10^{19} cm^{-3}$, respectively. The peak intensity wavelengths are obtained as 363.17nm for GaN and 845.7nm for GaAs.

خلاصة البحث

يوضح هذا العمل تأثير تعاطي المنشطات على بنية نطاق الطاقة لطبقات الصمام الثنائي الباعث للضوء المتجانسة. ويربط هذا البحث القيم الناتجة عن طاقة فجوة النطاق ومنطقة استنفادها، التي يتم تطبيقها بعد ذلك على طيف التلألؤ للصمام الثنائي الباعث للضوء. وتتم محاكاة بنية نطاق الطاقة من خلال تهيئة خصائص المواد المختلفة لنتريد الغاليوم (GaN)، بما في ذلك زرنيخيد الغاليوم (GaAs)، وحل معادلة بواسون المشتقة من معادلة النقل بولتزمان عن طريق تطبيق طريقة الفروق المحدودة وطريقة نيوتن-رافسون. وتتم مقارنة كلتا المادتين بتركيزات مختلفة من المنشطات في النطاق من 1×10^{18} cm^{-3} إلى 1×10^{21} cm^{-3}. ويتم التحقق من صحة هيكل الفرقة الطاقة مع النتائج الأدب من خلال اتخاذ خصائص السيليكون كمتغير التي تسيطر عليها. تنتقل طاقة فجوة النطاق المقاسة لـ-GaAs من 1.4273 eV إلى 1.4640 eV ، ومن 3.3970 eV إلى 3.4148 eV بالنسبة لـ-GaN. وتزداد طاقة فجوة النطاق مع نسبة زيادات تركيز المنشطات. ومع ذلك، إنه ينخفض من (1.5700×10^{-1} ميكرومتر – 7.5000×10^{-3} ميكرومتر) ومن (1.8450×10^{-1} ميكرومتر – 8.5000×10^{-3} ميكرومتر) × 1 ميكرومتر على التوالي عند الحصول على المناطق المكانية D-1 النشطة للطبقة فوق المحورية لـ-GaAs و GaN. وتظهر النتائج أن تركيز المنشطات مشبع عند عتبة معينة، مما يوفر تأثيرًا أقل أهمية على بنية نطاق الطاقة لأشباه الموصلات. وبالتالي، يحدد النظام العددي طيف خرج LED والقيم الحدية لطاقة فجوة النطاق. وتم الحصول على عتبات فجوة النطاق التي تم تحليلها في 1.440 eV لـ-GaAs و 3.403 eV لـ-GaN بتركيزات المواد من 2.951×10^{19} cm^{-3} و 4.467×10^{19} cm^{-3} على التوالي. وتم الحصول على أطوال موجات شدة الذروة على أنها 363.17 نانومتر لـ-GaN و 845.7 نانومتر لـ-GaAs.

APPROVAL PAGE

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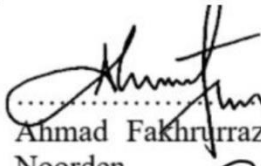

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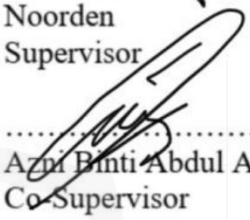

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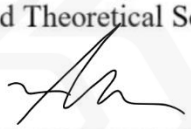

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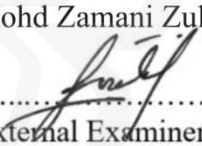

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For the one and only True God

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General current density equation	$J(x) = e\int vy(v,x)\,dv$	18
Drift-diffusion of electrons	$J_n = qn(x)\mu_n E(x) + qD_n\frac{dn}{dx}$	19
Drift-diffusion of holes	$J_p = qp(x)\mu_p E(x) - qD_p\frac{dp}{dx}$	19
Diffusion current	$J(r) = qc\mu E(r)$	19
Drift current	$J(r) = -qD\frac{dc}{dr}$	20
3-dimensional drift-diffusion	$J = qc\mu E + qD\nabla \mathrm{c}$	20
1-dimensional, carriers' rate of change in volumetric epitaxial region	$Adx\frac{\partial y}{\partial x} = J_c(x+dx)\frac{A}{q} - J_c(x)\frac{A}{q} + (G_n - R_n)Adx$	20
Rate of change of current density	$J_c(x+dx) = J_c(x) + \frac{\partial J_c}{\partial x}$	21
The flux of carriers through a single node of surface area	$\frac{dc}{dx} = -\frac{1}{q}\frac{\partial J_c}{\partial x} + (G_c - R_c)$	21
General flux expression	$\frac{\delta c}{\delta t} = \frac{1}{q}\nabla.\overrightarrow{J} + U_c$	21
Electrostatic Poisson's equation	$\nabla.\epsilon\nabla V = -(p_0 - n_0 + N_D - N_A)$	22
Scahfetter-Gummel discretization		

	$J_{i-1/2}^{j} = \frac{qD}{\Delta}\left[n_i B\left(\frac{V_i - V_{i-1}}{V_T}\right) - n_{i-1} B\left(\frac{V_{i-1} - V_i}{V_T}\right)\right]$	23
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LIST OF SYMBOLS

A	Area	π	pi
B	Bernoulli's function	R	Residual form
c	Charged particle	R_c	Recombination constant
D	Diffusion constant	R	Depletion region
∇	Differential	φ	Fermi potential
ϵ	Dielectric constant	T	Temperature
E	Energy	t	Time
e	Exponential	V	Electric potential
G	Generation constant	v	Velocity of particle
h	Plank's constant	ω_p	Well-defined plasma edge
I	Intensity		
J	Current density		
k_B	Boltzmann's constant		
k_F	Wave vector		
ln	Natural logarithm		
μ	Mobility of carrier		
m^*	The effective mass of a particle		
N	Density of states		
n	Electrons concentration		
p	Hole concentration		
q	Particle's charge		

LIST OF ABBREVIATIONS

Al	Aluminum	Ge	Germanium
BE	Bandagap Energy	HEMT	High Energy Mobility Transistor
DDM	Drift Diffusion Model	In	Indium
DR	Depletion Region	LED	Light-Emitting Diode
EBS	Energy Band Structure	LS	Luminescence Spectrum
FDM	Finite Difference Method	Si	Silicon
GaAs	Gallium Arsenide	SRH	Shockley Read Hall
GaN	Gallium Nitride		

CHAPTER ONE

INTRODUCTION

1.1 RESEARCH BACKGROUND

As the modernized lighting technologies that produce environmental-friendly illumination are globally demanding, realizing the physics behind them undoubtedly benefits humankind and mother nature. Lighting technology has evolved from illumination based on the electron thermal agitation mechanism known as incandescence to the electrons transition mechanism, known as luminescence (Derenzo, 2003). Respectively, some of the well-known examples of lighting devices are torches, candles, and tungsten lightbulbs, fluorescent tubes (MacIsaac et al., 1999), and the semiconductor light-emitting diodes (LED) (Y. K. Cheng & Cheng, 2006).

The semiconductors are widely applied to high energy mobility transistor (HEMT), LED, laser diodes, and solar cells (Denbaars et al., 2013; Fletcher & Nirmal, 2017; Gobat et al., 1962; Metaferia et al., 2019; Shealy et al., 2002). Various numerical simulations have been performed to analyze the semiconductor materials' doping effect, mechanism, and performance (Datta, (2005), and Pisarenko and Ryndin, (2019). They describe the carriers' transport mechanisms with their formulation modelings in detail. The numerical analysis is recently focused on the thermoelectric properties, the effective mass of carriers, and piezo-polarisation effects (Misra et al., 2020; Sirkeli et al., 2015a; Wu et al., 2020; X. Zhang et al., 2019).

The EBS overviews the semiconductor material's valence and conduction bands, including the bandgap energy, which is essential. Commonly, most of the carriers'

dynamical mechanism is connectively analyzed via its energy band structure (EBS). Otherwise, it can be deductively concluded via its efficiency calculations, such as the internal and external quantum efficiencies (Shaari et al., 2020; Zhu et al., 2009). Several reports show the enhancement of semiconductor performance can be achieved by inducing doping (Asl & Rozati, 2020; Egerton et al., 2005; Hao et al., 2019; Yi et al., 2006). The compatible doping concentration towards a *p* or *n*-types material will produce desirable optical and electrical properties useful for specific applications (Dewan et al., 2017; Egerton et al., 2005). However, the dopants' concentration optimization requires extensive numerical simulation works, including the drift-diffusion model (DDM) and EBS theory.

The DDM has been widely used in previous works of literature for analyzing and solving the problem in the semiconductor field (Lundstrom, 2015; Sujecki, 2014a; Vasileska et al., 2017). However, the incompatible dopant concentration infused affects the semiconductor to behave like the non-semiconductor, leading to an incorrect estimation of the desired luminescence spectrum. Another issue is that bandgap energy's and depletion region's correlation with the EBS affected by the dopant concentration is still ambiguous.

In this research, the DDM is performed by approximating the semiconductor chip layers to a homogenous media, altering the dopants concentration, and imposing conditions at the boundary of the epilayer with 0 and bias potential at the start of *n*-type and at the end of *p*-type semiconductor. The model is used to analyze the performance of the GaN- and GaAs-based LED in a homojunction vertical chip configuration. The analysis is performed based on the effective mass of carriers (electrons and holes), the bandgap energy, and the depletion region of the semiconductor. Lastly, the validation

is executed by estimating the luminescence spectrum of both LEDs and compare it with literature findings.

1.2 PROBLEM STATEMENT

Doping in semiconductors helps to reduce the potential energy required for electrical conduction to occur between the electrodes. Yet, an extensive amount of the dopants' concentration affects the properties of the semiconductor, thus changing it to behave as the non-semiconductor. Non-semiconductor, which are the conductors and insulators, have distinct nature of EBS to the semiconductor. Inaccurate EBS causes the incorrect model of chip's output spectrum. Besides, the doping process affects the bandgap energy and depletion region of a semiconductor as well. Thus, the correlation of these properties with the EBS is still vague which can affect the numerical estimation of the light properties produced by a LED chip. The dynamic correlation between dopant concentration aand luminescence spectrum is still unclear which requires a comparative study and analysis across different materials. Eventually, the incompatible dopants concentration infused in semiconductor material leads to incorrect estimation of the desired luminescence spectrum.

As an analogy, one desires to produce a specific-colored light, with the help of dopants in semiconductors, one expects to improve the energy efficiency. But, unfortunately, the LED color is shifted to a different wavelength beyond the visible range. The worst case is that it would not make any light of any wavelength at all as it has converted to a non-semiconductor.

1.3 RESEARCH OBJECTIVES

The research is mainly focused on investigating the effect of dopant concentration on the LED performance. The specific objectives include:

1) To apply the drift-diffusion model equations in creating a numerical simulation script for the EBS simulation of homojunction LED chip.
2) To correlate the bandgap energy and depletion region with dopants concentration through Newton's Raphson method.
3) To compare the effects of dopant concentration on GaN and GaAs-based homojunction LED chip in terms of bandgap energy and depletion region.
4) To simulate and analyze the output luminescence spectrum of LED chips based on the EBS.

1.4 RESEARCH QUESTIONS

1) What are the mathematical theories involved in estimating the energy band structure of the homojunction LED using DDM.
2) What is the relationship between the bandgap energy and depletion region to the dopant concentration?
3) 2) What effects of dopant concentration changes are different between GaN- and GaAs-based semiconductors?
4) 3) How the luminescence spectrum of LED change with the heavily doped semiconductor epitaxial layers?

1.5 RESEARCH HYPOTHESIS

This research has predicted results as the following hypotheses:

1) The EBS of GaAs and GaN will differ significantly from each other since both emit different spectrums.
2) There will be a threshold of dopants concentration for enhancing the bandgap energy of the homojunction epilayer.
3) The output wavelength of GaAs and GaN-based epilayer will shift with the increment of dopant concentration.

1.6 RESEARCH SCOPE

This research is conducted to develop numerical programming for EBS simulation. The solution of the modeled simulation covers the mathematical theories of Newton Raphson's method, Poisson's equation, current equation, and drift-diffusion equation. Deriving from EBS, this research focuses on the doping effects in LED epitaxial layers visualized via their luminescence spectrums and supported by their bandgap energy and depletion region values.

The effect of doping is considered for heavy dopants concentration in basic LED material. The concentration values are chosen from $1x10^{18}$ cm^{-3} to $1x10^{21}$ cm^{-3}. The epitaxial layer configuration follows the vertical LED chip where the electrodes are connected vertically. The LED epitaxial layers dimension is set with 1x1x1 μm^3. The complex equations are approximate by linearization to 1-dimension to compensate for the time and high-end hardware requirement for 3-dimensional simulation.

CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION TO SEMICONDUCTOR

The semiconductor can be defined as the material that can conduct electricity if applied with specific minimum electrical potential (0-15 eV), according to Dittmer et al. (2019), providing enough energy for their valence electrons to break free (Zhang et al., 2019). For example, germanium (Ge) and silicon (Si) - elements with single valence electrons, or Gallium Nitride (GaN) and Gallium Arsenide (GaAs) - the combinations of two or more elements. These combinations of two elements are called binary semiconductors (Kurchin et al., 2018), where the *p*-type semiconductor is made up of element with holes (unoccupied states in the valence shells) and the *n*-type that consists of the element with extra valence electrons (Meyer et al., 2012).

Combining elements made up of group-3 and group-5 (III-V) from the periodic table will produce stable state valence electrons. More of such semiconductor studied by Akiyama et al. (2009), Bhuiyan et al. (2003), Dayeh (2010), and Kazan et al. (2007) are Aluminum Nitride (AlN), Indium Arsenide (InAs), Indium Nitride (InN) and the rest are shown in Figure 2.1. Yet, as Campbell et al. (2012) have clarified, two of the most common combination of group III-V are the GaAs and GaN.

In the world that we are living now, semiconductors are found everywhere in computer systems (Cheng & Cheng, 2006; Hart & Estrin, 1991), transportation advancements (Ndiaye et al., 2016; Shamsi et al., 2013), communication technologies (Abarbanel et al., 2001; Vrijen & Yablonovitch, 2001), lighting(Berencén et al., 2011;

Haitz & Tsao, 2011), sensing (Rothberg et al., 2011; Toumazou et al., 2013), etc. Modernized technologies have developed numerous semiconductor configurations to enhance the overall efficiency. Heterojunctions and heterostructures semiconductors are hot topics in the current semiconductor research. Such works were conducted by Schultz et al. (2021), Wang et al. (2019), Yang and Hao (2019), Zhang and Jaroniec (2018).

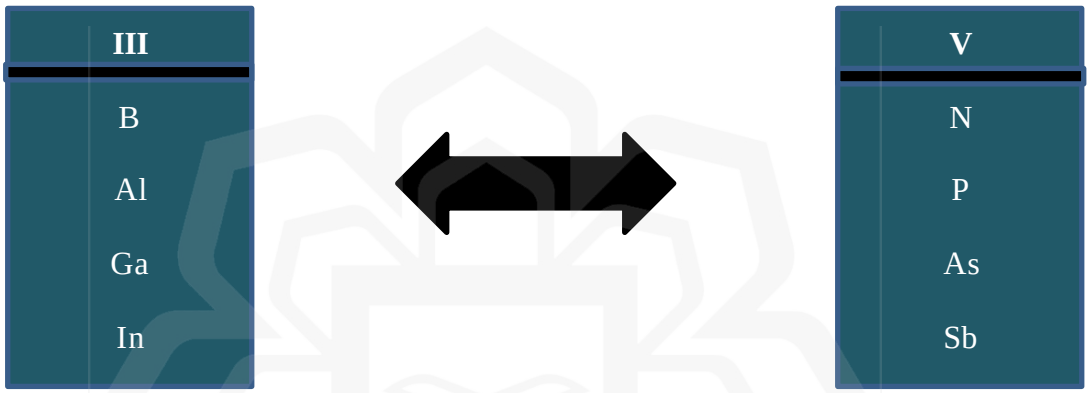

Figure 2.1. Group III-V semiconductor combinations

2.2 DOPING IN SEMICONDUCTOR

One of the earliest techniques to increase efficiency for basic binary semiconductors is by doping the semiconductor material. Doping is adding extrinsic carriers into the pure semiconductor (Gupta et al., 2017; Manyala et al., 2008). Such carriers come from impurity element that is compatible with the intrinsic semiconductor. The element that is compatible with the group III-V semiconductor comes from the same group.

Aluminum (Al) and Indium (In) are both compatible with GaAs and GaN. Works by Burgess et al. (2016), Malguth et al. (2008), Pradhan et al. (2017), Yılmaz et al. (2017) configure such compatible configurations as the dopants for enhancing the group III-V semiconductors. On the other hand, Man (1971) and Piprek (2012) found that