Simulation of high performance quantum well GaN-based LED

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ABSTRACT

The performance of quantum well GaN/AlGaN light emitting diode (LED) is reviewed for three different barrier compositions, symmetric barrier composition with low Al content, asymmetric barrier composition with higher Al content on p-type cladding layer and lower Al content on n-type cladding layer, and symmetric barrier composition with higher Al content The study was conducted using ATLAS/BLAZE & LUMINOUS software developed by Silvaco International Inc Integrated radiative recombination rate was studied on applied voltages up to 5V Results showed three phases of LED performance with different applied voltages and these were explained using bandgap theory I-V characteristic for each design agrees with the total additional voltage drop equation for a quantum well structure The dominant radiative recombination rate regions in LED at low and high supplied voltages are also presented for the best performance LED design

Keywords GaN, LED, quantum well, radiative efficiency, conduction band, valence band, I-V characteristic

1. INTRODUCTION

An LED is a compound semiconductor device that emits visible or infrared light when an electron current passes through it It contains a p-n junction with a direct transition band structure Injected electrons and holes recombine near the p-n junction area to emit light In order to increase light emitting efficiency, a double hetero-junction structure is widely used, which is made by sandwiching an active layer by p-type and n-type semiconductor layers that have larger band gaps The wavelength of the emitted light is determined by the band gap of the semiconductor material in the active layer

GaN and its related materials have been widely used as candidate materials for the realization of visible or ultraviolet (UV) laser diodes (LDs) and light emitting diodes (LEDs) [1] Major developments in the GaN-related materials have recently led to the commercialization of high-brightness blue, green and ultraviolet LEDs and to the realization of violet LDs with a lifetime of more than 10,000 h [2 5] Recently, the UV light source is attracting considerable attention for the application to excite various kinds of florescent materials and also the application in medical equipments, communication equipments detectors sensors and other field [3] As demonstrated by GaN related optical devices, many device structures such as GaN/AlGaN, InGaN/GaN and InGaN/AlGaN must take advantage of quantum wells (QWs) Thin quantum wells LED devices offer the potential of higher injected carrier densities and hence more efficient radiative recombination Thin active layers also serve to minimize self-absorption in LEDs with relatively low internal quantum efficiencies, which is important in device structures wherein photons make multiple passes through the active layer before escaping from the LED [6] Generally, tight carrier confinement gives strong influence on LED performance Here the mechanism and optimization of barrier composition balance play an important role in order to achieve a higher carrier confinement in active layer especially Simulation is an inexpensive, faster and relatively easy tool that can offer many results to explain the characteristics of LED It is also a practical tool that can be used to make comparisons between different LED structures in order to achieve higher performance of LED

In this paper, we investigate GaN single quantum well active region with cladding by different barrier composition of $Al_xGa_{1-x}N$ The radiative efficiency for each design for different applied voltages from 0V to 5V is reviewed The results are explained using conduction band and valence band diagrams The investigations on I-V characteristics for different barrier composition of LED design are also performed The results obtained were different compared to a bulk system where current output increases as the radiative efficiency becomes higher in bulk system The inverse result was achieved in quantum well structure in which the variation of voltage drop in quantum well gives effect on LED performance The distribution of radiative recombination concentration regions for the best performance LED design is also presented

2. SIMULATION PROCEDURES

Simulation was carried out using ATLAS/BLAZE & LUMINOUS software developed by Silvaco International Inc BLAZE accounts for the effect of positionally dependent band structure by modifications to the charge transport equations which simulated the LED performance The bandgap difference distribution between the conductance and valence band has a large impact on the charge transport in these heterodevices The affinity rule method is used by default to define the conduction band and valence band alignments for a heterointerface LUMINOUS was used with BLAZE to extract certain parameters associated with light emitting devices This allows the simulator to extract luminous efficiency by dividing the integrated radiative recombination rate (radiative efficiency) with total integrated recombination rate This simulator is incorporated with radiative recombination models like Shockley-Read-Hall (SRH), Quantum, Auger, Optical and Bandgap narrowing model SRH model specifies Shockley-Read-Hall recombination using fixed lifetimes while Quantum model enables activation of quantum moments model Auger specifies Auger recombination, which occurs through a three particle transition whereby a mobile carrier is either captured or emitted[7] Optical recombination model was modeled in this form,

$$R_{opt} = C_{opt}\,(n\,p - n_i^{2}) \tag{1}$$

where C_{opt} – 3x10^{11} cm^{3}/s is a constant value for GaN[8]
Bandgap narrowing model is important in heavily doped region Bandgap narrowing effect may be described by an analytic expression relating the variation in bandgap, ΔEg to the doping concentration[7] From Fig 1, light emission mostly resulted from active region Emitted light is in the **z**-direction (normal to page) Hence, the integrated radiative recombination rate will be in the form of emission in **z**-direction per width

Fig 1 shows the 2-D mesa structures of GaN based LED with different barrier composition balance structures that have been simulated in this work First cladding layer was p-type AlGaN with Mg doping concentration of 1 5x10^{17} cm^{3} followed by p-type GaN active layer which was doped with 5x10^{16}cm^{3} Mg Their thicknesses are 100 nm and 50 nm respectively Doping concentration of silicon at 5x10^{18}cm^{3} was applied on n-type AlGaN with thickness of 100 nm GaN Si n-type acts as substrate with doping concentration of 5x10^{18} cm^{3} and thickness of 2μm These structures were supplied by forward biases from 0 1V to 5V

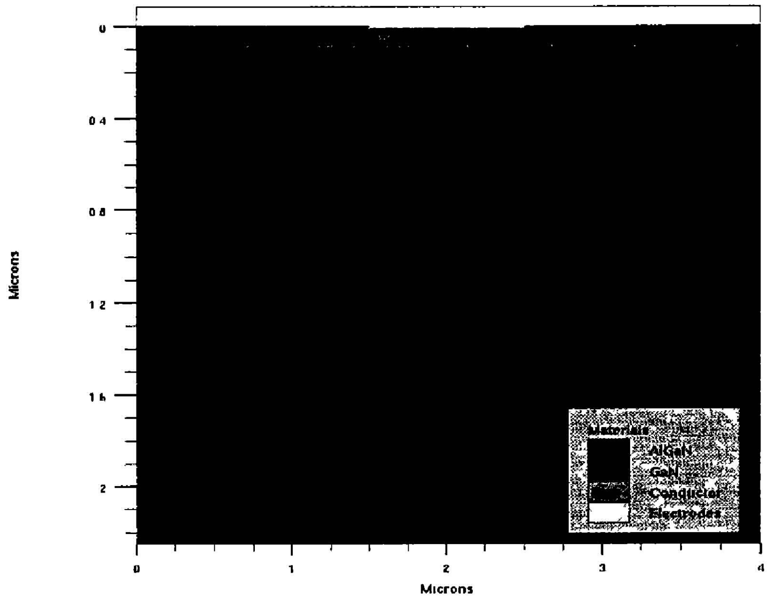
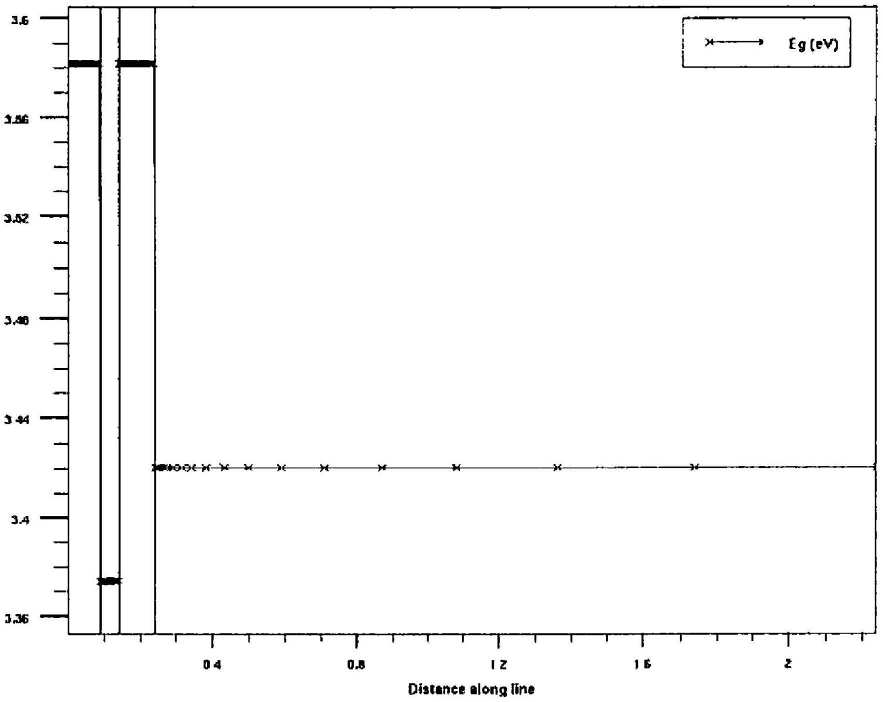
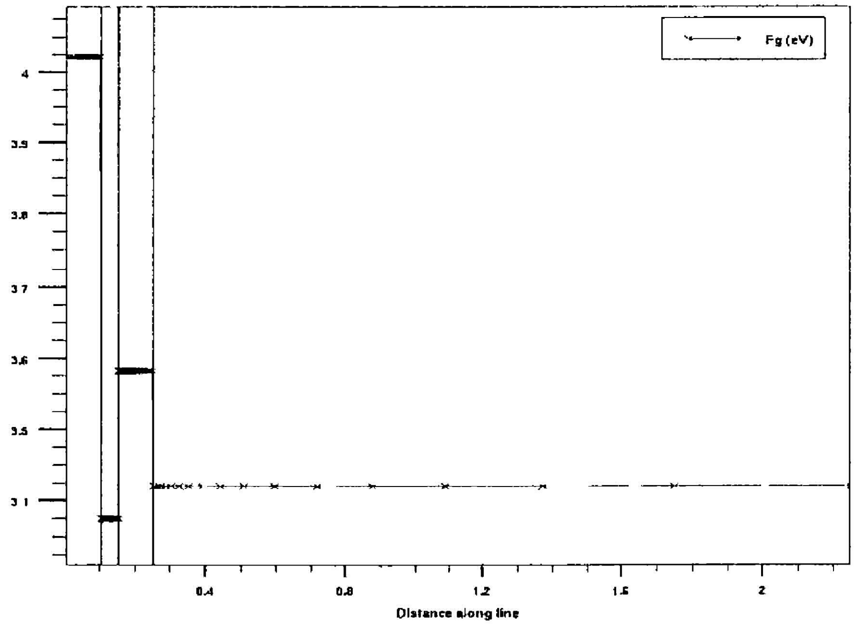


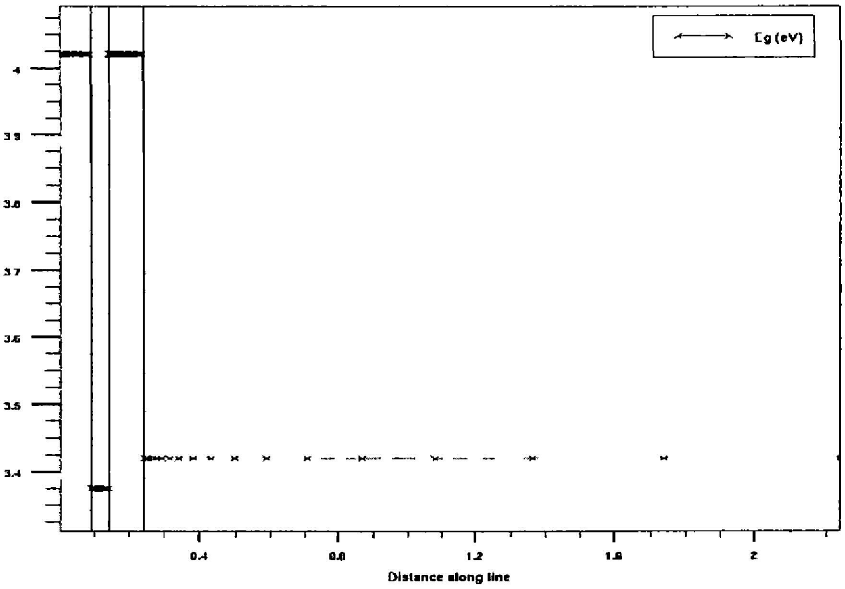
Fig 1 The 2-D mesa structure of GaN based LED



(a) symmetric barrier with Al content at 0.09



(b) assymmetric barrier with Al content at 0.3 on p-type AlGaN and 0.09 on n type AlGaN



(c) symmetric barrier with Al content at 0 3

Fig 2 The 2 D mesa structure of GaN based LED with different barrier composition balance (a) p type Al $_x$ Ga $_{1 x}$ N and n-type Al$_x$Ga $_{1 x}$ N with x - 0 09 (b) p type Al $_x$ Ga $_{1 x}$ N with x = 0 3 and n-type Al$_x$ Ga$_{1 x}$ N with x - 0 09 (c) p type Al $_x$ Ga $_{1 x}$ N and n type Al $_x$Ga $_{1 x}$ N with x = 0 3

3. RESULT AND DISCUSSIONS

Sec 3.1. Integrated radiative recombination rate versus voltage

Fig 3 indicates integrated radiative recombination rate versus the applied voltages Apparently, radiative efficiency increase as the applied voltage increases for these designs and give three different behavior on LED performance For a symmetric structure with low Al content of 0 09, (structure (a)) highest radiative efficiency is achieved at 0 1V but there are fluctuations for structure (b) and (c) at below 2 2V The performance of all LEDs at 2 2V until 3V is almost similar for the different designs with structure (c) producing highest output compared to structure (b) and (a) Lastly, for further applied voltage above 3V, structure (b) contributes to the highest radiative efficiency followed by structure (a) and structure (c)

H X Wang et al 2004 [9], presented that at low Al content composition, symmetric barrier shows a higher confinement that can give higher performance at low injection current and a larger carrier spill over at higher injection current The asymmetric barrier composition showed a large leakage at low injection current which may be caused by the barrier compositions changing from symmetry to asymmetric thus, the leakage current would be increased [9] but it manages to achieve a better performance at higher injection current The symmetric barrier with high Al content composition gives the highest performance at both low and high voltage supply since it can decrease the carriers spill over and also increase the confinement of carriers in the active region

At very low voltage supply, structure (b) gives the lowest performance, possibly due to the changing of barrier composition from symmetric to asymmetric which leads to higher leakage current [9] At voltage range from ~0 5V to ~1 8V, the radiative efficiency in structure (b) becomes higher than structure (c) due to the reduction of leakage current in structure (b) compared to structure (c) However, for applied voltages between ~1 8V to 2 2V, structure (c) gives higher performance than structure (b) because of increase in barrier confinement which leads to better confinement of carriers compared to structure (b) At this condition structure (a) still gives highest radiative efficiency because of lower barrier found in this structure

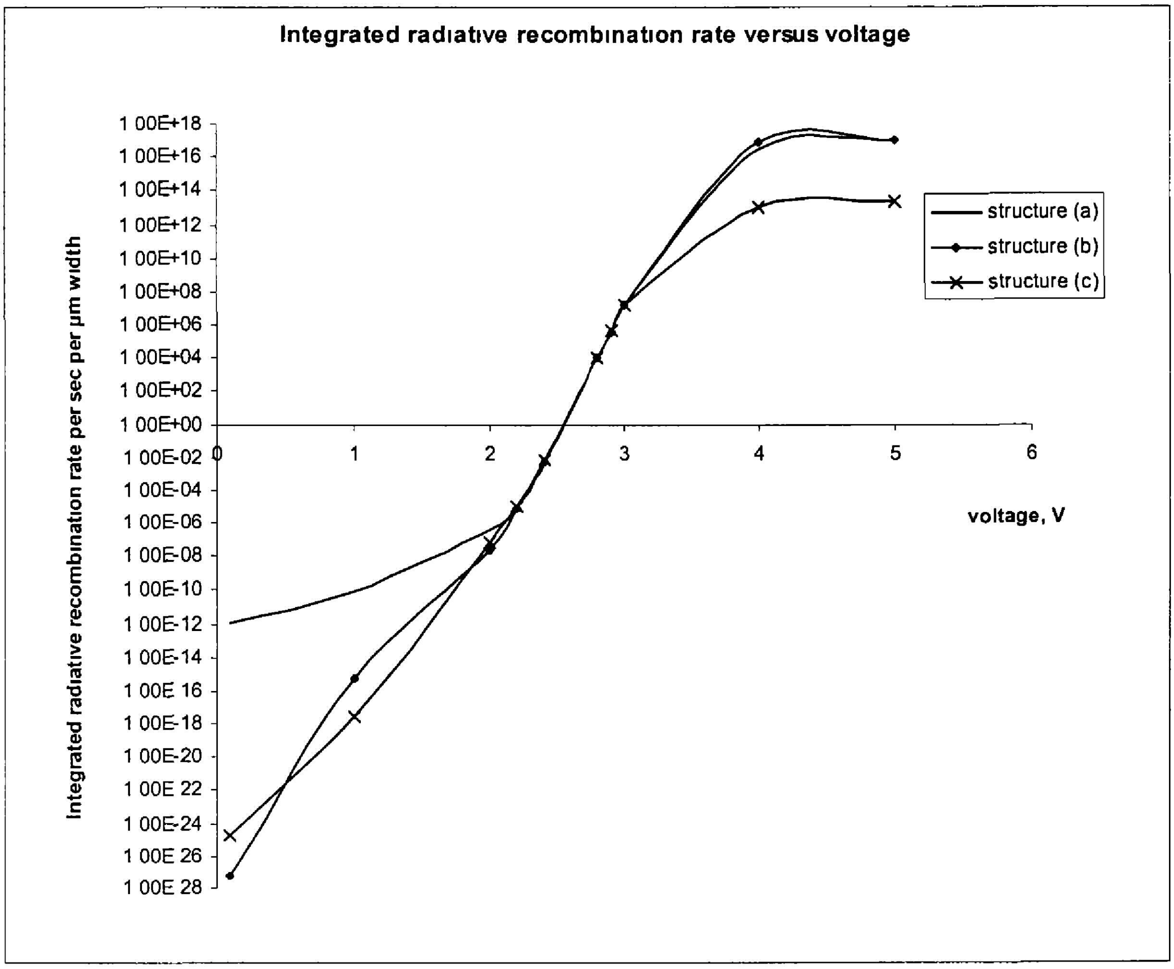
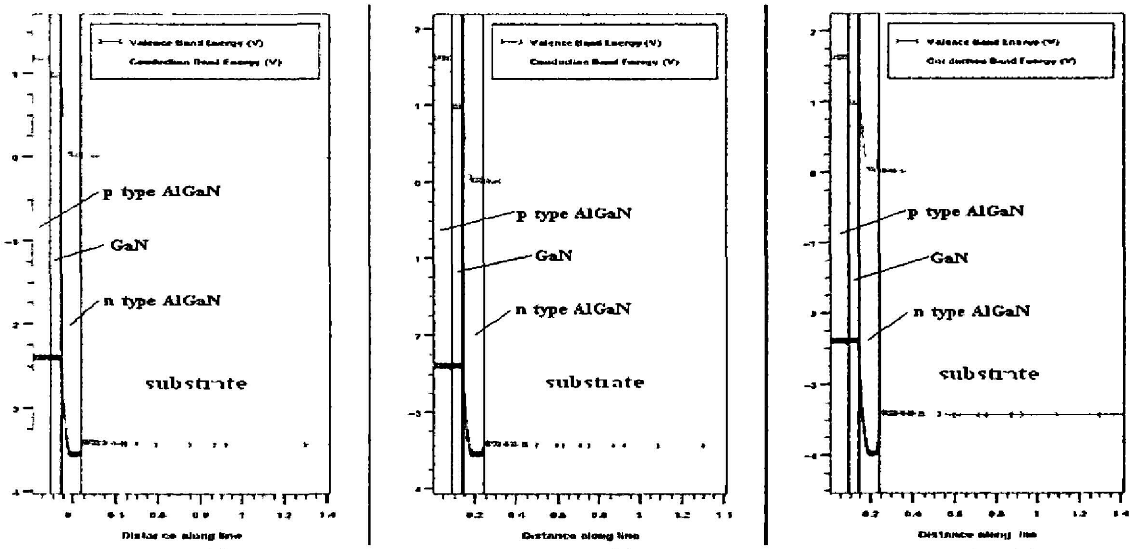


Fig 3 Integrated radiative recombination rate versus applied voltage for three LED structures

Based on Fig 3, all the structures give almost the same radiative efficiency at 2 2V to 3V However, by referring to Fig 4, the highest barrier (1 225V) at GaN/n-type AlGaN interface cladding layer had been found at conduction band in structure (c) However, at this supplied voltage, electrons may have enough energy to overcome this barrier The better confinement of electrons owing to the highest barrier at p-type AlGaN/GaN results in less electrons spilling over the barrier and diffusing into the cladding layer The highest band discontinuity at p-type AlGaN/GaN in structure (c) provides a good confinement of carriers Generally, at low voltage supply, overflow of carriers is not dominant and there are unoccupied states for the carriers in the quantum well active region A good confinement is required to impede carriers' diffusion into cladding layer

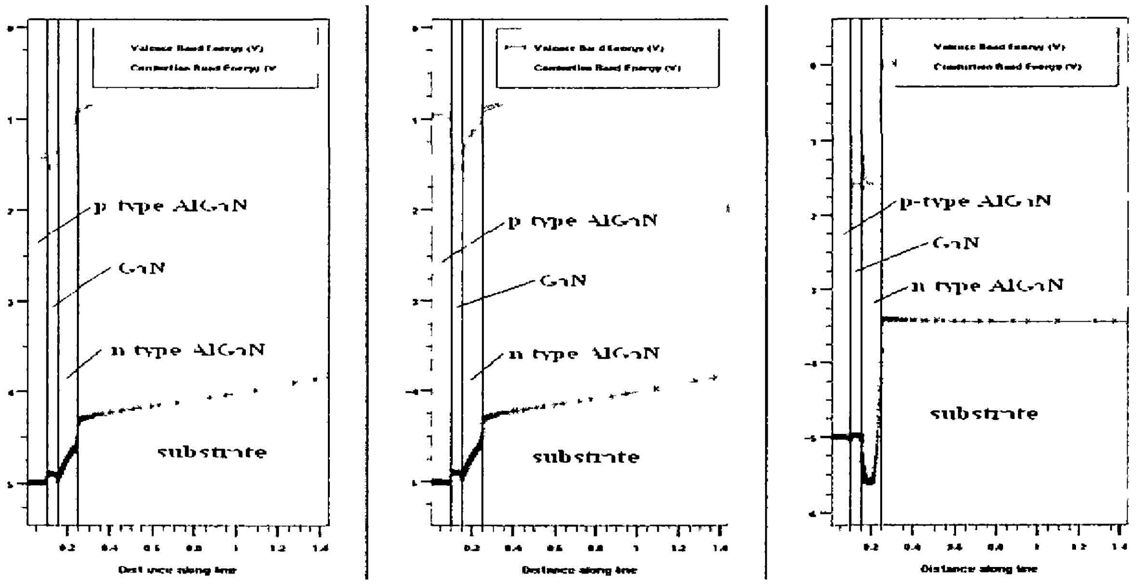
Clearly, when the supplied voltage is at 5V, there is no barrier at GaN/n-type AlGaN interfaces in the conduction band for structures (a) and (b) except in structure (c), as shown in Fig 5 Hence, more carriers are able to be injected into the active region easily Spill-over occurs less in structure (b) compared to structure (a) due to a higher barrier at p-type AlGaN/GaN interface In structure (c), there is a barrier at GaN/n-type AlGaN interface and carriers spend a longer time to overcome this barrier This mechanism will increase carriers' lifetime and loss of energy before they are confined in the active region From detailed observation of the valence band, holes tend to overflow over p-type barrier in structure (a) compared to structure (b) due to higher barrier obtained in structure (b) The higher barrier was formed at GaN/n-type AlGaN interface in structure (c) but lowest barrier was attained at p-type AlGaN/GaN interface Thus, spill over of holes into p-type AlGaN/GaN interface is greater in this structure

Here, we suggest that lower barrier at GaN/n-type AlGaN interface gives an advantage compared to lower barrier at p-type AlGaN/GaN interface at conduction band The overflow of electrons into n-type AlGaN cladding layer leads to the possibility of electrons being injected into GaN active region again These electrons have an opportunity to make recombination with holes and increase radiative recombination of the LED



structure (a) structure (b) structure (c)

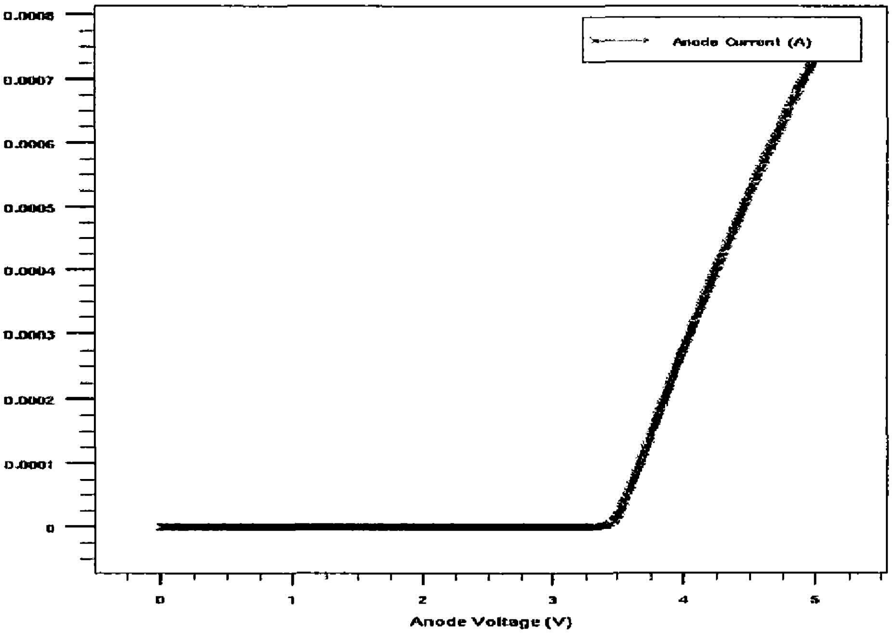
Fig 4 The conduction band and valence band diagram for three designs at 2 4V



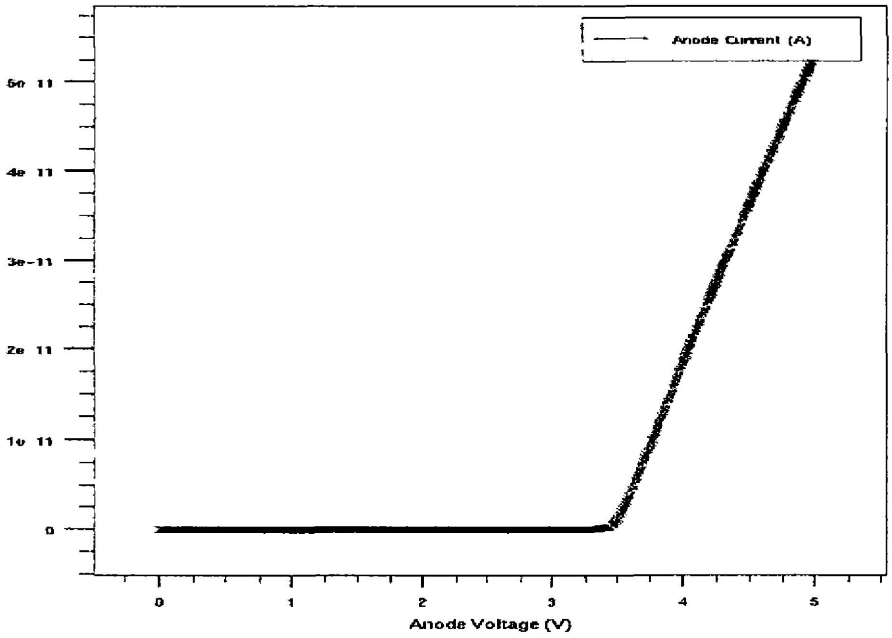
structure (a) structure (b) structure (c)

Fig 5 The conduction band and valence band diagram for three designs at 5V

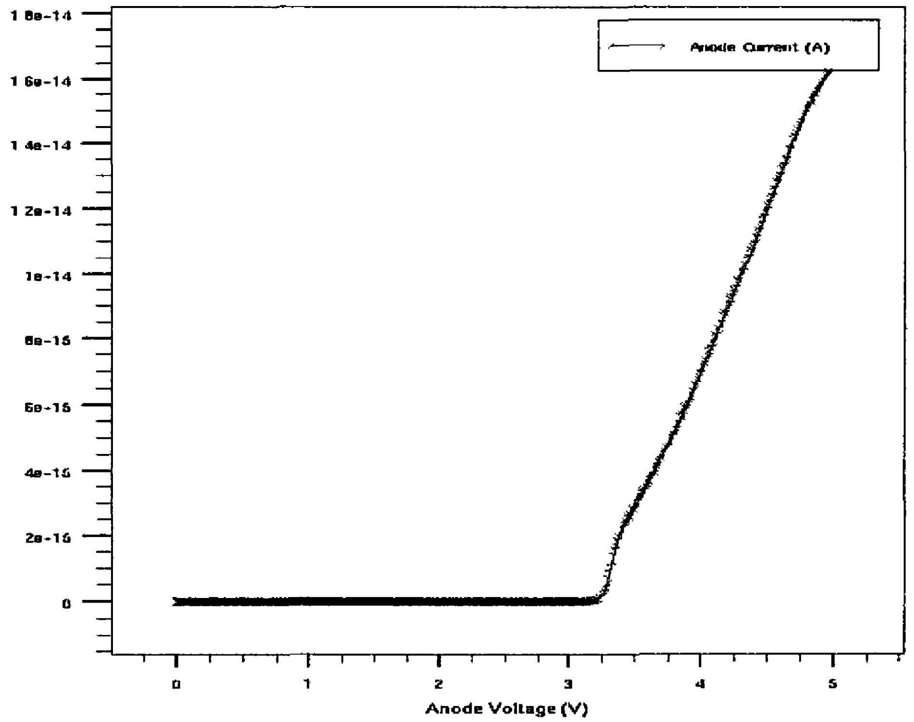
Sec. 3.2: Anode current versus anode voltage



a structure (a)



b structure (b)



c structure (c)

Fig 6 Anode current versus anode voltage for three structures (a) (b) and (c) At 5V Fig 8a shows anode current occurs at 0 734 mA while Fig 8b shows anode current occurs at 5 26x10^{8} mA Fig 8c shows anode current occurs at 1 64x10^{11} mA

Fig 6 shows anode current versus anode voltage for three structures Structure (a) performs with the highest output current followed by structure (b) and finally structure (c) Generally, voltage drop occurs when diode has a significant series resistance The additional series resistance can be caused by several factors such as contact resistance, bulk resistance particularly in materials with low carrier concentrations or low carrier mobility, and resistances caused by abrupt heterostructure In this work first and second factor are constant for these LED designs, however the third factor contributes to the current output since at 5V there are formations of barrier at GaN/n type AlGaN in structure (c) The carrier energy may be reduced upon injection into a quantum well structure or double heterostructure causing an additional voltage drop as well Upon injection into the quantum well, the electron loses energy ΔE_c E_0, where ΔE_c is the band discontinuity and E_0 is the energy of the lowest quantized state in the conduction band quantum well Similarly, the energy lost by holes is given by $\Delta E_v - E_0$, where ΔE_v is the band discontinuity and E_0 is the energy of the lowest state in the valence band quantum well Upon injection of carriers into the well, the carrier energy is dissipated by phonon emission The energy loss due to non-adiabatic injection of carriers is relevant in semiconductors with large band discontinuities [10] Based on the following equation, the total voltage drop across a forward-biased LED is given by

$$V = \frac{E_g}{e} + IR_s + \frac{\Delta E_c - \Delta E_o}{e} + \frac{\Delta E_v - \Delta E_o}{e} \qquad (2)$$

From equation (2), total voltage drop increases as the band discontinuity ΔE_c and ΔE_v are increased Hence, since structure (a) has the lowest ΔE_c it gives a higher output current , followed by structure (b) and structure (c) The symmetric structure with high Al content (structure (c)) has higher additional voltage drop due to high series resistance and largest band discontinuity, ΔE_c and ΔE_v , hence producing lowest output current

Sec.3.3: The distribution of radiative recombination concentration

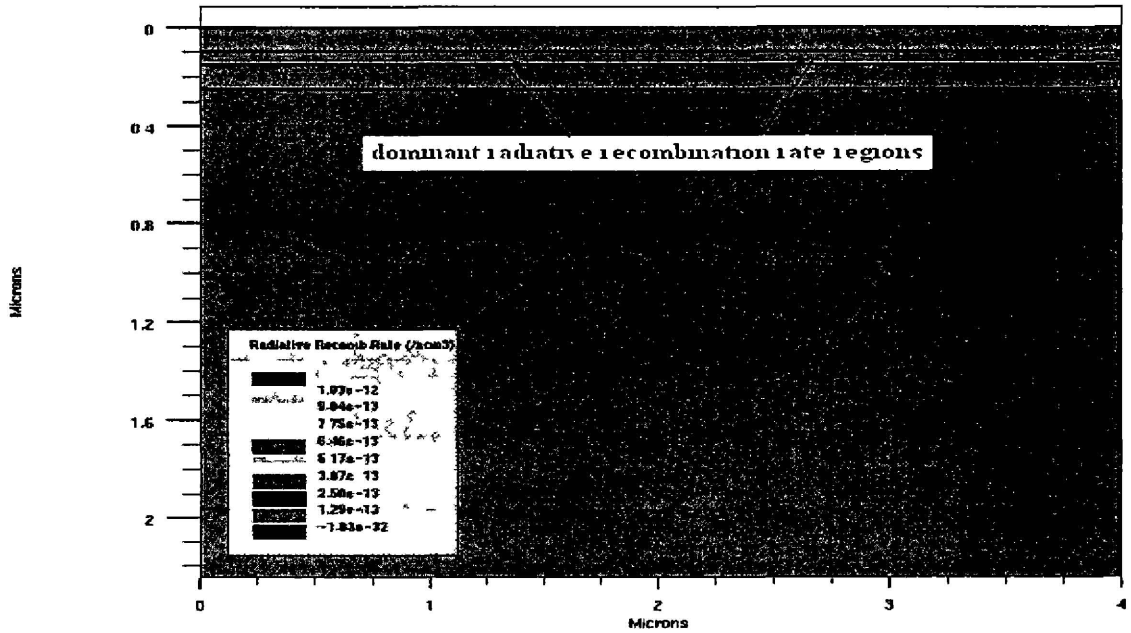


Fig 7 The distribution of radiative recombination concentration region at 0 1V for structure (b)

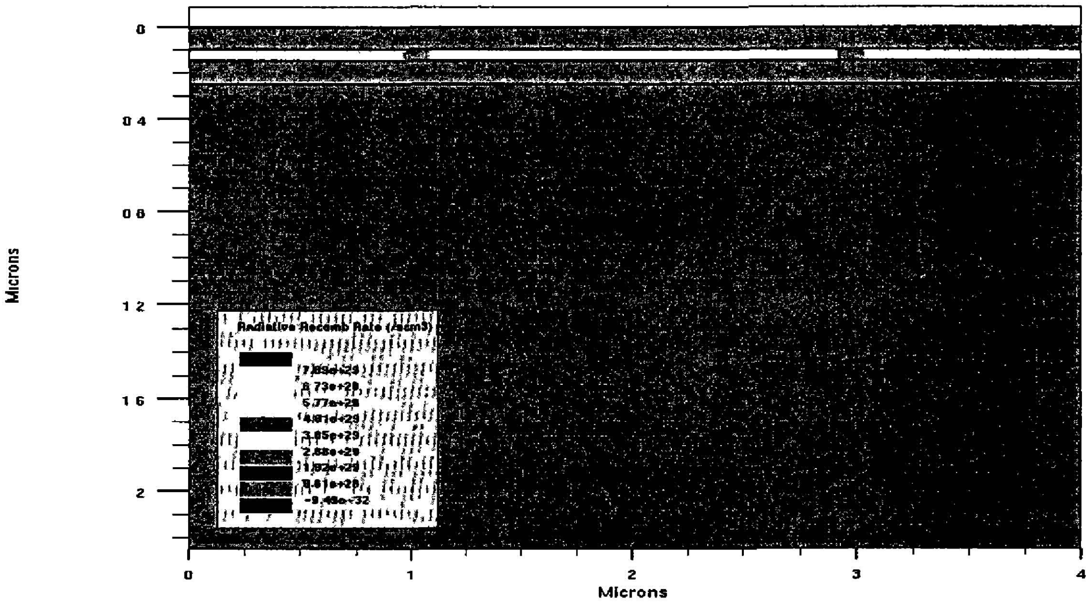


Fig 8 The distribution of radiative recombination concentration region at 5V for structure (b)

Structure (b) produces the best performance for voltages of 0 1V and 5V respectively, and the distributions of its dominant radiative recombination regions are shown in Fig 7 and Fig 8 At low injected voltage, dominant radiative recombination regions are dominant at certain areas in GaN active region The radiative region becomes larger when the voltage is increased It reveals an increase in the recombination events of electrons with holes that lead to an increase in light emission More light emission leads to enhancement of radiative efficiency

4. CONCLUSIONS

At very low voltages, structure (b) (asymmetric barrier composition) gives the lowest performance due to higher leakage current For voltages between ~0 5V to ~1 8V, structure (b) gives better performance due to decrease in leakage current For further applied voltages, (~1 8Vto 2 2V), structure (c) (symmetric barrier composition with higher Al content) shows better performance because of better confinement of carriers However, structure (a) (symmetric barrier composition with low Al content) still gives the highest performance at voltages below 2 2V At 2 2V to 3V, all the structures produce almost similar performances At higher injection voltage, structure (b) displays the best performance due to good confinement at conduction and valence band Although structure (c) seems to have better confinement than structure (b), there are barrier formations at GaN/n-type AlGaN interfaces at cladding layer which leads to lower radiative efficiency Current output results agree with the total voltage drop equation for quantum well structure The current output is reduced with large band discontinuity at conduction and valence band At very low voltages, the distributions of dominant radiative recombination regions are dominant at certain regions in active region, while the distribution of dominant radiative recombination regions covers almost the entire active region at higher voltages

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