Available online www.ejaet.com

European Journal of Advances in Engineering and Technology, 2014, 1(2): 39-50

Research Article

ISSN: 2394 - 658X

Theoretical Investigation of Highly Efficient ZnO Heterostructure-based Bluish Light Emitting Diode

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ABSTRACT

A comprehensive numerical analysis has been accomplished for ZnO system based double heterostructure visible light emitting diode (LED) with superior electrical and optical performances. The optimized device with thin active region of CdZnO layer having 15% composition emits bluish electroluminescence around 430 nm, at room temperature with device internal quantum efficiency (IQE) of ~70% at anode current 0.22A. Rigorous theoretical investigation has been performed for the device parameter optimization; more specifically optimization of device barriers and cap layers along with active region. The optimization involves thickness, doping, and alloy composition calibrations of various constituent layers. Different aspects of band gap engineering and confinement has been considered to identify the optimization criteria for the design of ZnO based LEDs.

Key words: Bluish ZnO LED, double heterostructure, electroluminescence, quantum efficiency

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INTRODUCTION

Recently there has been profound interest in ZnO and its alloys while realizing high performance visible and ultra violet (UV) light emitting devices. The ZnO has a direct band gap of 3.37 eV at room temperature, a high free-exciton binding energy of 60 meV, relatively low material cost and long-term stability [1]. Compared to its group III-N counterparts, ZnO possesses advantages including higher quantum efficiency, greater resistance to high-energy radiation, availability of high-quality substrates [leading to simple vertical light-emitting diodes (LEDs) geometries], and the ability to use wet chemical etching [1,2]. The band gap Eg linearly increases with x up to 4.15 eV for 0< x< 0.36 while still maintaining the wurtzite structure [3] and saturates at higher Mg concentrations due to MgO segregation. This indicates that MgxZn1−xO is a suitable material for barrier layers in ZnO/ MgZnO hetero structures with a band-gap offset up to 0.85eV [4,13]. Similarly, Cd incorporation in ZnO results in the reduction of band gap energy since CdO (2.3 eV) has smaller band gap. To achieve a broader range of emission wavelengths, ZnCdO active regions have been considered essential due to the controllability of band gap. Thus, we designed double heterostructure system with CdZnO active region [5]. There are several reports [6-8] on the growth of heterostructure materials to form LEDs; however, in all those cases, the hetero-interfaces had to accommodate a large lattice mismatch in the interface of the constituent layers; that on the other hand has greatly compromised with the device performance. Dislocations formed at the device interface as a result of strain generally form non-radiative defects that can seriously reduce the quantum efficiency of LEDs [9]. The realization of band gap engineering to create barrier layers in heterostructure devices is critically important in the design of such ZnO-based heterostructure LEDs. Here we adopted all ZnO layers approach on silicon substrate. Several parameters have been considered for the heterojuntion device designed for 430 nm emission wavelength. The double heterostructure device increases the carrier density in the radiative recombination region by confining the carriers in the active region, thus resulting in an enhancement of the light emission.

ZnO material system-based blue LEDs are attractive due to their high brightness and high-power capability in lighting and display applications. Reliable and highly efficient blue light emitting diodes are in high demand for daily uses [8]. Methods for maximizing the efficiency of light emitting diodes typically fall into two categories.

The first is to improve the efficiency of light emission in the active region, or the internal quantum efficiency (IQE). The second method is to increase the ratio of photons leaving the LED to those created in the active region, or the external quantum efficiency (EQE) [9]. We have put our emphasis on internal quantum efficiency by optimizing the design parameters to enhance the radiative recombination rate in the device active region. Fig.1 presents the cross-sectional view of the device studied in this paper.

In this paper, the device modelling and numerical simulation for the ZnO-based heterostructure LED in terms of constituent layer structure, doping and composition and their effect on light emission from the device and its threshold behaviour is thoroughly examined. This paper is divided into five sections. Section two describes the heterostructure device under consideration, detailing the layer characteristics considered for IQE optimization, and summarizes the material models employed in the simulations. This section is further subdivided into five parts to discuss the design tradeoffs for the electron and hole blocking layers, effects of active region thickness and cap layers performance parameters on device IQE. Section third emphasized on the band gap engineering for hetero junction devices. Section fourth presents the design issues approach and analysis of simulated results. Finally, conclusions are discussed in last section.

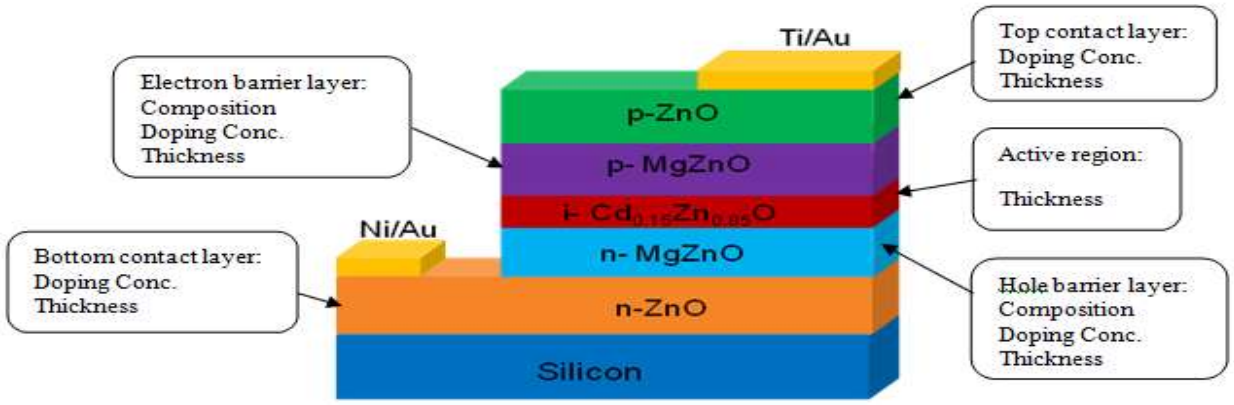


Fig.1 Cross sectional view of the considered LED structure, outlining the regions whose parameters has been optimized in order to achieve the maximum IQE

DEVICE STRUCTURE

On top of the substrate, an n-type ZnO layer is deposited and this layer behaves as a bottom contact layer. An n-type MgZnO layer is grown on the top of bottom contact layer which will act as a barrier for holes. In the heterostructure device, the $Cd_{0.15}Zn_{0.85}O$ layer is considered to be the active region. An electron barrier layer of MgZnO remains on the top of CdZnO active region, and this layer will act as a current spreading layer [10]. The top and bottom barrier layers have lower index of refraction thus they confine light by reflections at interfaces. Finally, the structure is completed with a top p-type ZnO contact layer. Au/Ti and Au/Ni were taken as anode and cathode electrodes to make good ohmic contacts [11]. In the simulation the device width has been considered to be 1μm. The effect of thickness and doping concentration of contact layer on the device performance has been investigated. Furthermore the effect of barrier thickness, doping concentration, and composition, on the behavior of the device has also been studied.

The device performance of heterostructure LED has been evaluated through the optical intensity which also gives photo generation rate. The intensity peak has been observed as a function of wavelength for uniform mesh density. The generation rate for a double heterostructure LED in terms of quantum efficiency is given by

$$G = \eta_0 \int_{\lambda max}^{\lambda min} P\lambda \frac{\alpha e^{-\alpha y}}{hc} \quad (1)$$

where η_o is internal quantum efficiency, λ_{min} and λ_{max} are spectral limits in terms of wavelength, P is ray intensity factor representing cumulative loss due to reflections, transmission etc in terms of wavelength, α is absorption coefficient of source, , h is Planck's constant and y is depth of device [12].

The extraction of the integrated radiative recombination in the device provides an estimate of luminous intensity. In order to extract luminous intensity, a luminous wavelength is specified in terms of wavelength parameter. The equation for luminous intensity (P) is:

$$P = \frac{hc}{\lambda} \int . R_{rad}\, dA \quad (2)$$

Where R_{rad} is radiative recombination coefficient and λ is wavelength [12].

The table I shows the material parameters required by the carrier transport equations, including the non-radiative, radiative, and Auger recombination coefficients, electron and hole mobilities and other additional parameters for ZnO based ternary alloys. In this device optimization, the composition of Cd in CdZnO has been kept fixed at 15%. All parameters were taken at room temperature [13], [14].

Table -1 Material Parameters used in the Simulation Study for the Binary and Ternary Alloys of Double Heterostructure LED

Parameters		ZnO	$Mg_xZn_{1-x}O$	$Cd_{0.15}Zn_{0.85}O$
Recombination lifetime	Electrons, n sec	1	6.5	1
	Holes, n sec	1	1	1
Radiative coefficient, $cm^3\ s^{-1}$		1.1×10^{-11}	2×10^{-11}	1.1×10^{-11}
Auger coefficient	Electrons, $cm^6\ s^{-1}$	1.0×10^{-34}	2.8×10^{-34}	1.0×10^{-34}
	Holes, $cm^6\ s^{-1}$	1.0×10^{-34}	1.0×10^{-34}	1.0×10^{-34}
	Permittivity	9	10.5	5.6
	Band gap, eV	3.37	4.1	3.0
Electron mobility	Minimum, $cm^2\ V^{-1}s^{-1}$	300	50	50
	Maximum, $cm^2\ V^{-1}s^{-1}$	2000	300	300
Hole mobility	Minimum, $cm^2\ V^{-1}s^{-1}$	5	1	1
	Maximum, $cm^2\ V^{-1}s^{-1}$	30	20	20

Optimization of MgZnO/CdZnO/MgZnO LED Structures

A heterojuntion is one of the key structures for constructing various electronic and optical devices using compound semiconductors. Modulation of band gap with keeping the lattice constants similar to each other is essential for this purpose. For instance, a double heterostructure (DH) composed of thin active region sandwiched between two barrier layers has been utilized for light emitting diode to facilitate radiative recombination by carrier confinement [15]. Since there is a crucial need of band gap tuning and optical confinement in heterostructure, optimization of process parameters for the ternary alloys is necessary in the design of optoelectronic devices. The conduction band edge up shift due to the effect of alloying Mg in ZnO causes an enhancement of activation energy and a reduction in the background carrier concentration. The optimal design conditions for the barrier layers are carried out for carrier and optical confinement to enhance the device performance. The MgZnO barrier layers play an important role for the design options in terms of device structures and selection of their relative design parameters with the goal of maximizing the IQE. For narrower band gaps, which are desirable for wavelength tunability and attaining band gaps corresponding to the visible spectrum, the CdZnO alloy has been preferred in most of heterostructure LED devices [16]. The transmittance increases up to 85% on increasing the Cd composition. The radiative recombination rate in a heterojuntion is given by $R_{rad} \sim C_{opt}$ np, where Copt is the radiative recombination coefficient and n and p are the excess electron and hole concentrations near the p–n junction interface, respectively. The realization of MgZnO and CdZnO ternary alloys rely on band gap engineering to provide carrier and optical confinement thus improves the efficiency of blue light-emitting devices and creates various application opportunities [16].

RESULT AND DISCUSSION

For each one of these layers, material parameters are optimized in order to best match the available device technology. We have determined an appropriate doping, molar concentration and thickness for the double heterostructure LED to achieve the highest possible IQE. The range of the various parameters used in this simulation study is summarized in Table 2. Following the methodology outlined in Table 1 we have considered the geometrical, composition and doping characteristics of each layer in the device simulation.

Table -2 Simulated Parameters used in Present ZnO based Double Heterostructure LED

Simulation conditions	Electron blocking layer	Hole blocking layer	Active region	Top contact layer	Bottom contact layer
Composition, %	0.1-0.3%	0.1-0.2%	0.15%	-	-
Carrier concentration, cm^{-3}	5×10^{16} - 5×10^{18}	5×10^{16} - 5×10^{18}	Intrinsic	5×10^{16} - 5×10^{18}	5×10^{16} - 5×10^{19}
Thickness, nm	50-400	50-500	30-200	50-100	50-500

ELECTRON BARRIER LAYER (EBL)

In the heterostructure LED, p-type MgxZn1-xO acts as the electron blocking layer. This layer acts as a barrier to prevent electrons to escape from the Cd0.15Zn0.85O active region. The intensity, threshold voltage characteristics (I-V), power spectra and quantum efficiency of the device structure is described with respect to alloy composition, doping concentration and thickness of the EBL. It has been noted that the other parameters of the device structure is held constant when any one of the parameter is varied.

Alloy Composition

Higher doping simply makes more holes available for recombining with electrons in the active region. It can be observed from Fig.2 that as we increase the Mg composition from 10% to 30%, there is a five-fold increment in emission intensity due to effective carrier confinement in the active region. The threshold voltage is reduced from 3.6 V to 3.3 V and power is increased from 0.07 W to 0.32 W on increasing the Mg composition which leads to the increase in quantum efficiency up to 60%. The thickness and doping concentration is fixed at 50 nm and 5×1016 cm-3 when the Mg composition is varied.

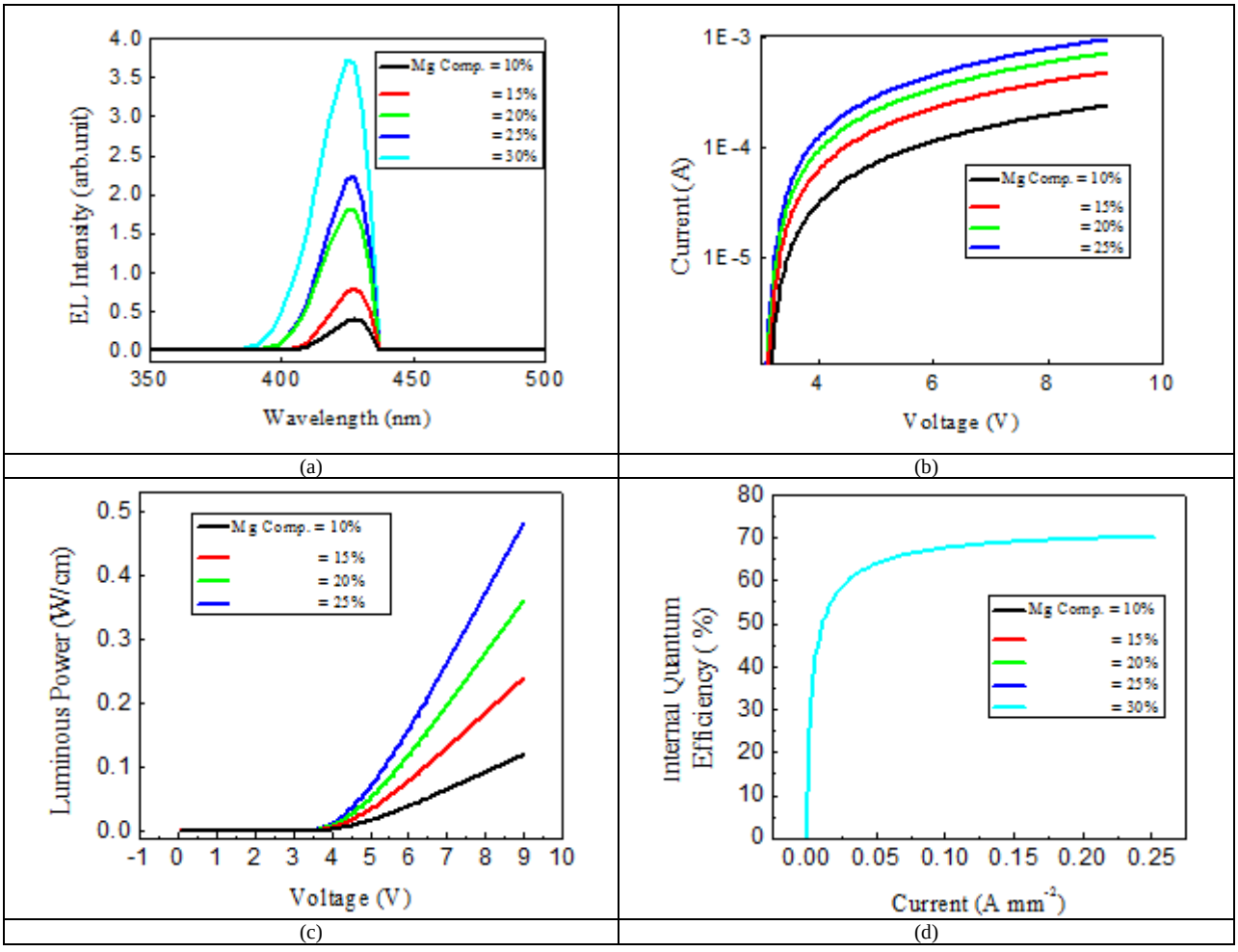


Fig. 2 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of Mg composition of the EBL layer of heterostructure LED

Doping Concentration

The doping level in the EBL is the second design degree of freedom in our device structure. It can be seen from Fig. 3 that the intensity shows a six-fold increment and luminous power increases from 0.12 W to 0.58 W with the acceptor doping concentration in the EBL. The threshold voltage also reduces from 3.6V to 3.3V as we increase the doping concentration (from 5×1016 to 5×1018 cm-3). The intensity had found to a minor impact on doping concentration. The composition and thickness is fixed at 10% and 50 nm when the Mg composition is varied.

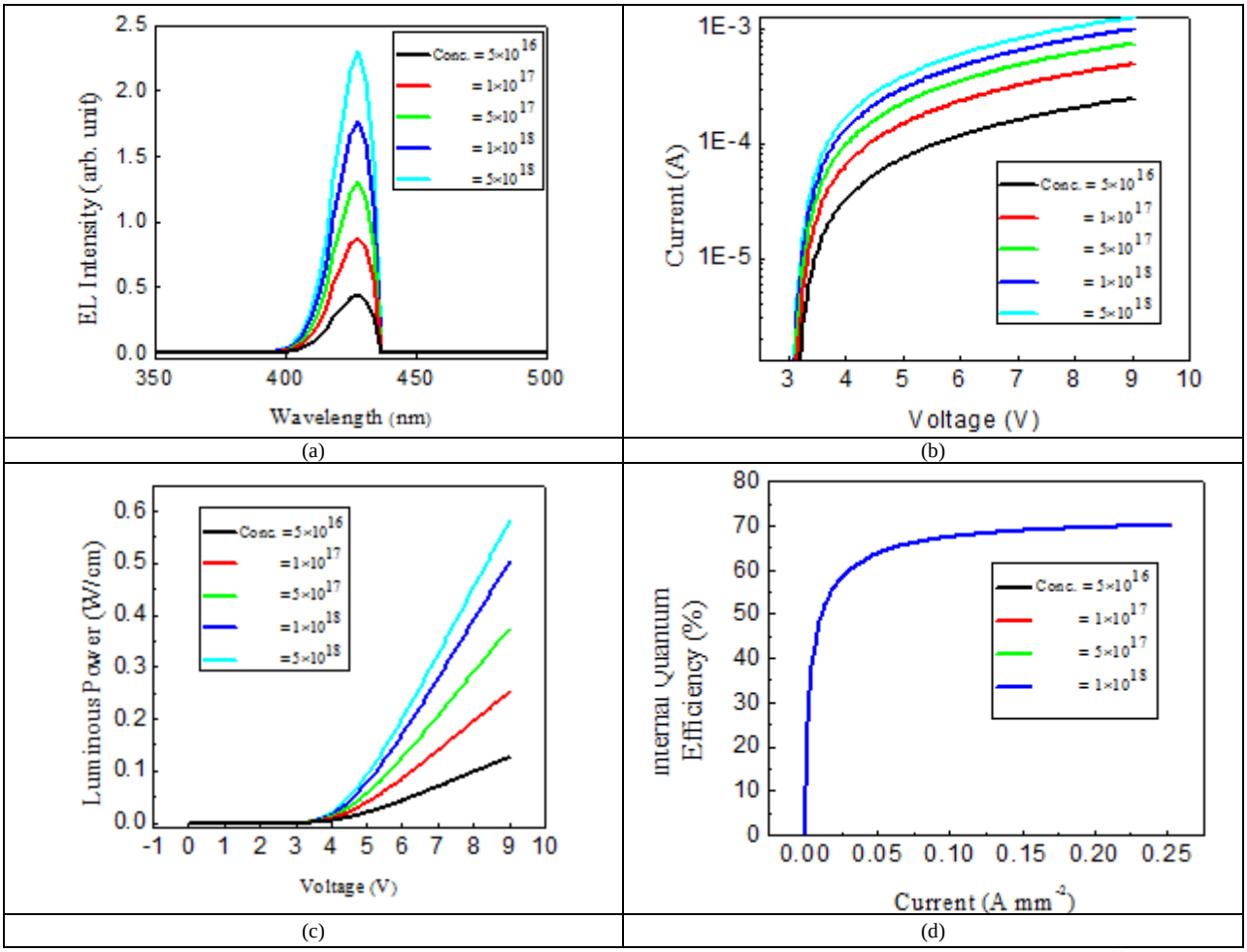
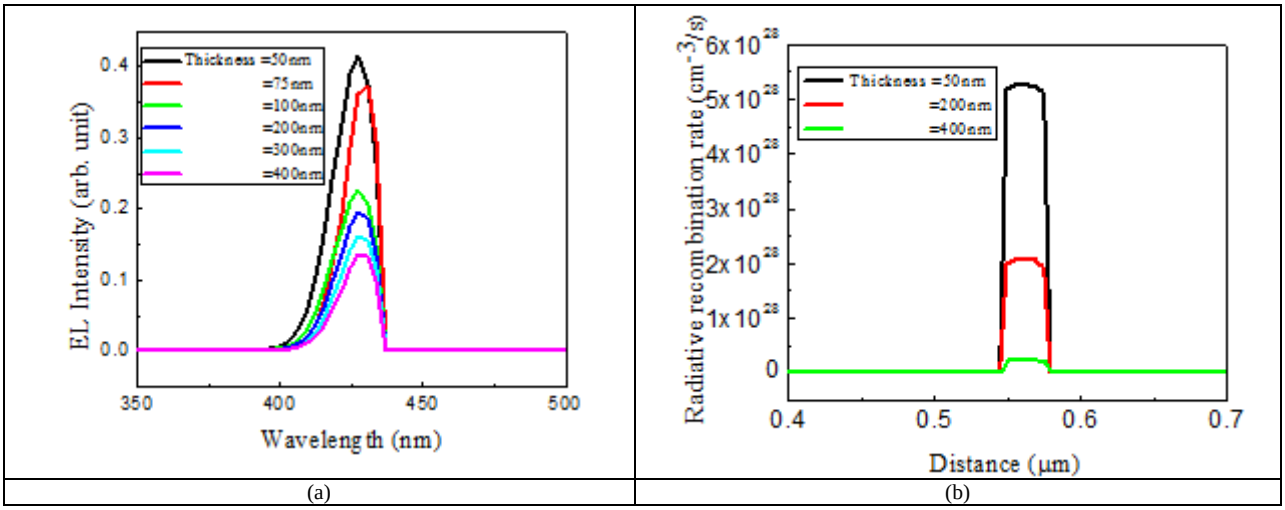
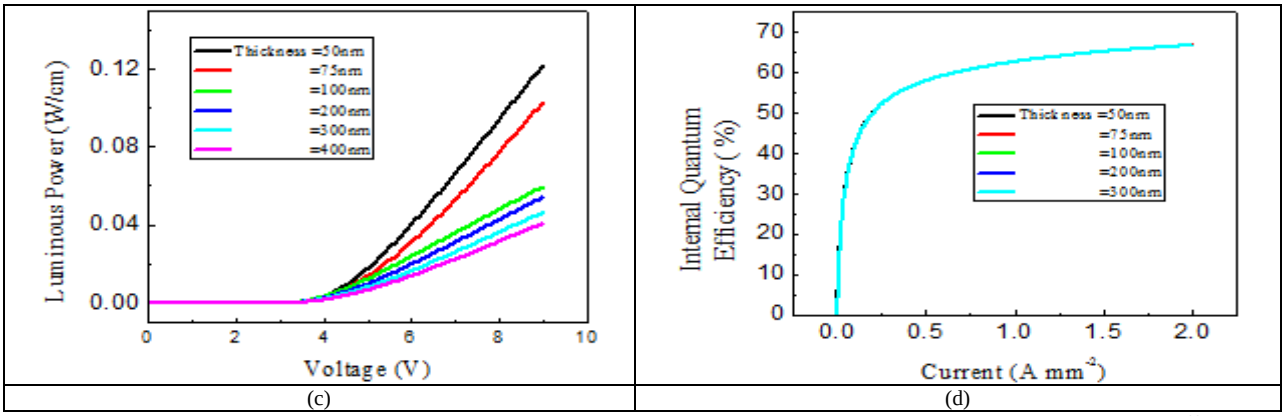


Fig. 3 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of hole doping concentration of the EBL layer of heterostructure LED

Thickness

The last device parameter in our structure of designing the EBL is its thickness. The current voltage characteristics shows increased device series resistance with the increase in thickness and this is illustrated by the degradation of threshold voltage from 3.4 V to 3.6 V when EBL layer thickness is increased from 50 nm to 400 nm (as illustrated in fig.3 (b) & (c). Secondly when the EBL thickness is increased, the radiative recombination rate decreases fivefold as a function of distance due to lowering of conduction band energy state. This may be due to native point defects such as zinc interstitials and oxygen vacancies, which leads the Fermi level to shift downwards in acceptor energy state [17].The doping concentration and composition is fixed at 5×1016 cm-3 and 10% when the thickness of EBL is varied.





(c) (d)

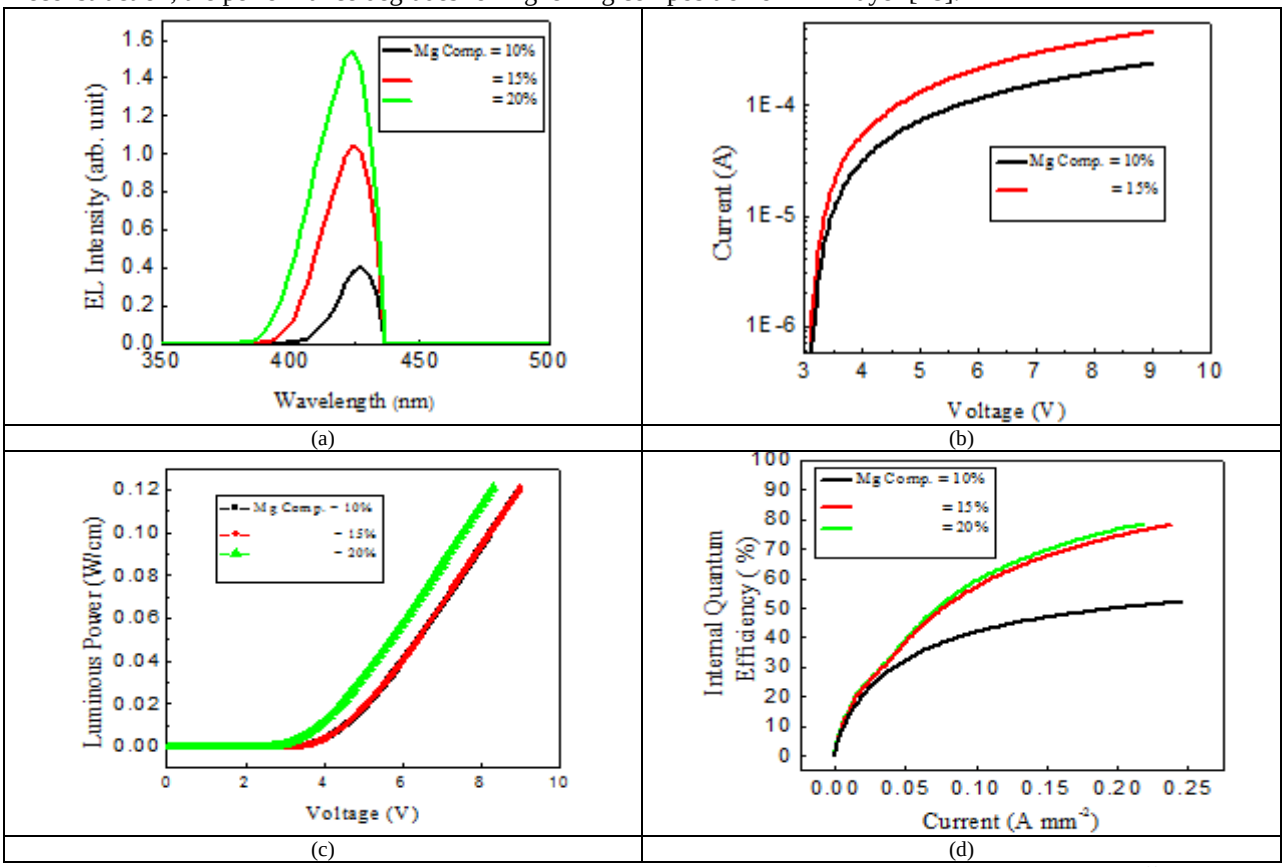
Fig. 4 Simulated (a) emission intensity spectra (b) I-V characteristic (c) radiative recombination rate and (d) internal quantum efficiency as a function of MgZnO layer thickness of the EBL layer of heterostructure LED

HOLE BARRIER LAYER (HBL)

Similar to the EBL optimization, the optimization of the hole barrier layer (HBL) is performed. This is essential in terms of maximizing device IQE, since suitable engineering of the HBL would ensure electrons in the active region resulting in the improved radiative recombination in the active region. For the HBL, as it has been done for the EBL in the previous section, we have considered the influence of alloy composition, doping, and thickness on the device IQE. It has been noted that the other parameters of the device structure is held constant when any one of the parameter is varied.

Composition

As seen from Fig.5, when the Mg composition is increased from 10% to 20%, the intensity shows a four-fold increment and threshold voltage also improves 3.3 V to 3.0 V which leads to increased quantum efficiency from 40% to 70%. The optimum Mg molar fraction has been kept constant at x = 15%. In ZnO-MgO ternary system, the thermodynamic solubility limit of MgO in ZnO is less than 4 mol% and due to heat induced band gap reconstruction, the performance degrades for higher Mg composition of HBL layer [18].



(a) (b)

(c) (d)

Fig. 5 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of Mg composition of the HBL layer of heterostructure LED

Concentration

It is seen from Fig.6 that as the electron doping concentration of the HBL layer is increased from 5×1016 to 5×1018 cm-3, a four-fold increment of electroluminescence (EL) intensity is observed. Since on increasing the doping concentration the carrier injection rate increases, the internal quantum efficiency improves from 50% to 60%. At this point, it should be noted that the thickness and composition of the HBL layer is held constant at 50 nm and 10% when its doping concentration is altered.

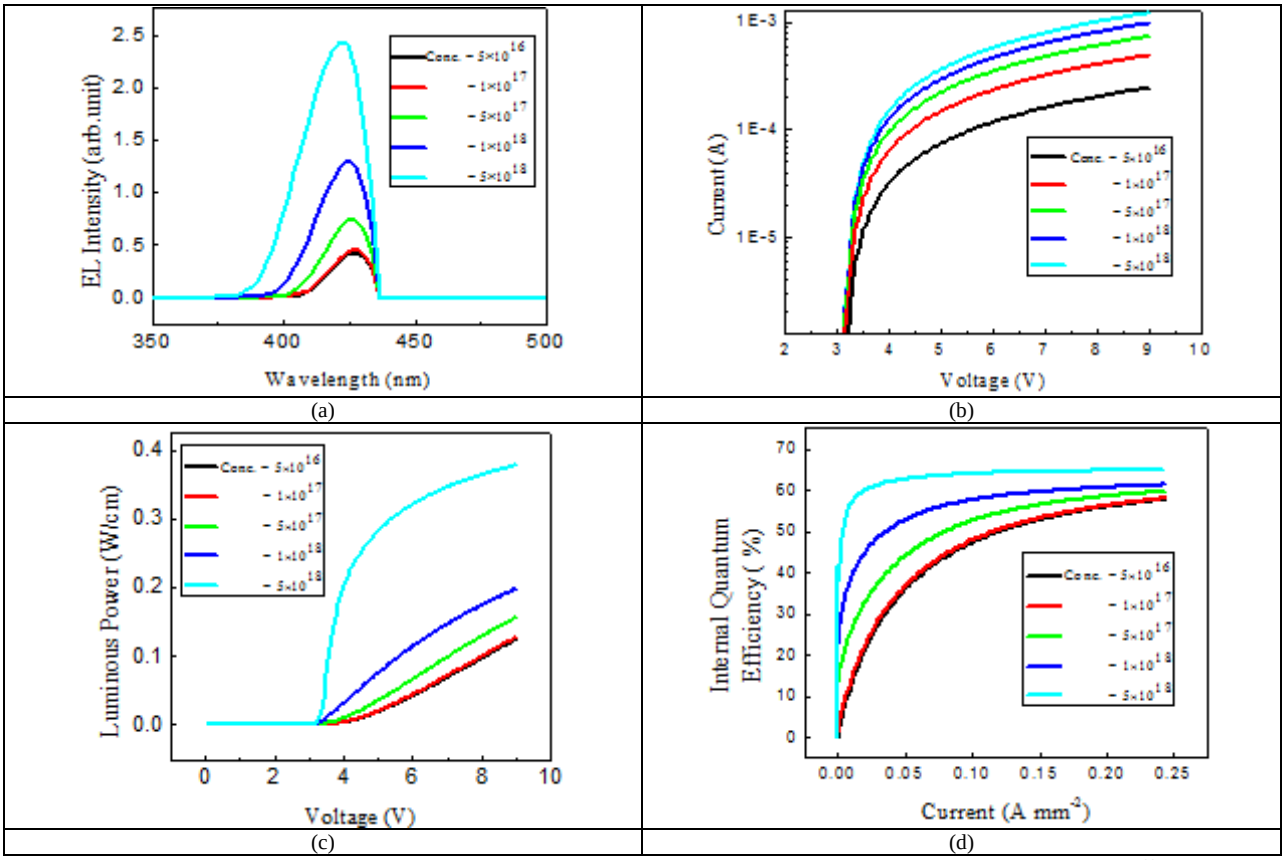
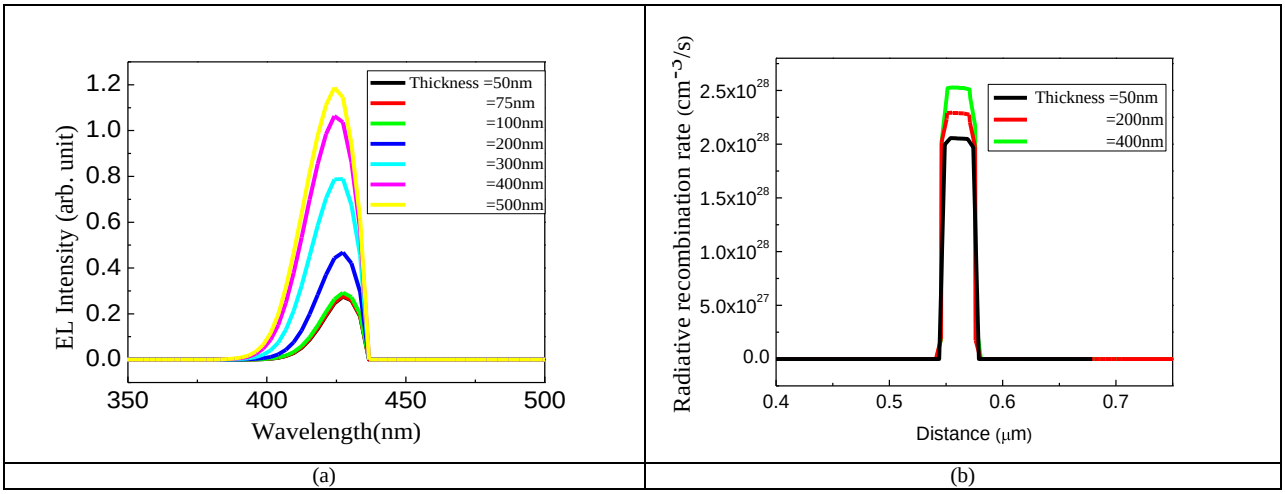
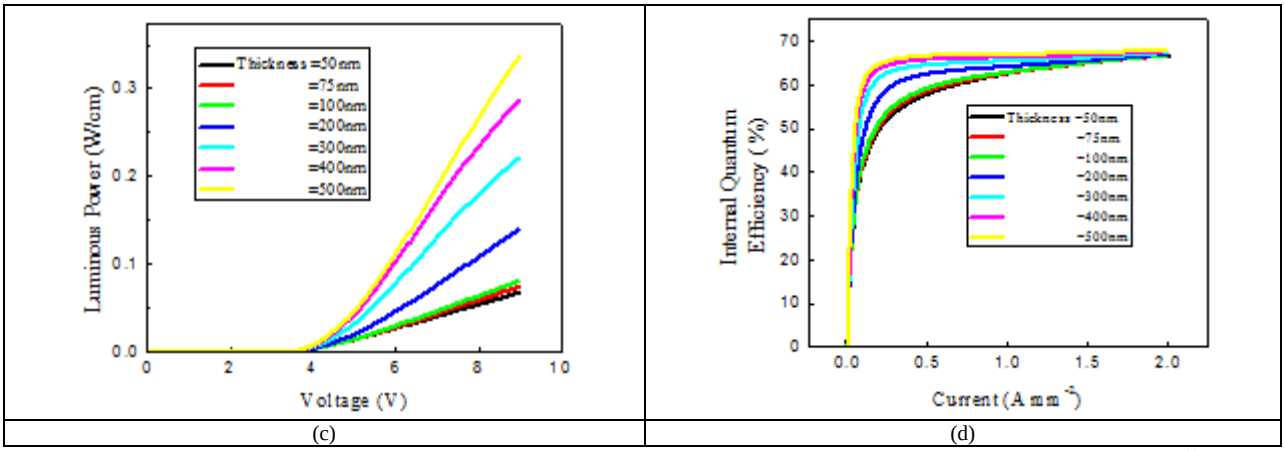


Fig.6 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of electron doping concentration of HBL layer of heterostructure LED

Thickness

From Fig.7 (a), it can be inferred that there is almost five-fold increment of peak emission intensity when the HBL layer thickness is increased from 50 nm to 500 nm. Similarly, the radiative recombination rate is increased from 2× 10^{28} cm^{-3}/s to 2.5× 10^{28} cm^{-3}/s and device threshold voltage (from 3.3V to 3.6V), is increased for the corresponding increase in the HBL thickness, as illustrated in Fig.7 (b) and 7 (c). The doping concentration and composition is fixed at 5×10^{16} cm^{-3} and 10% when the thickness of HBL is varied.



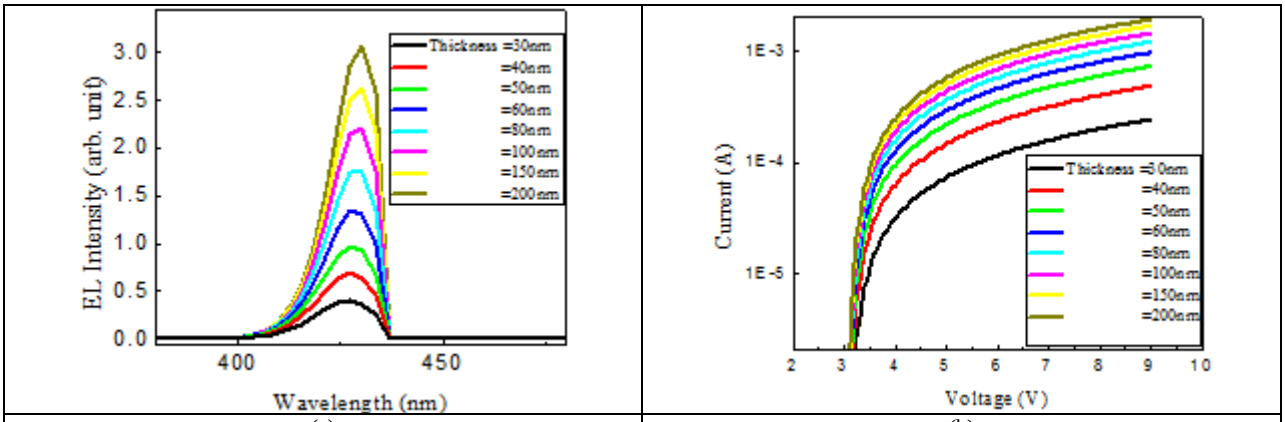


(c) (d)

Fig.7 Simulated (a) emission intensity spectra (b) I-V characteristic (c) radiative recombination rate and (d) internal quantum efficiency as a function of MgZnO layer thickness of the HBL layer of heterostructure LED

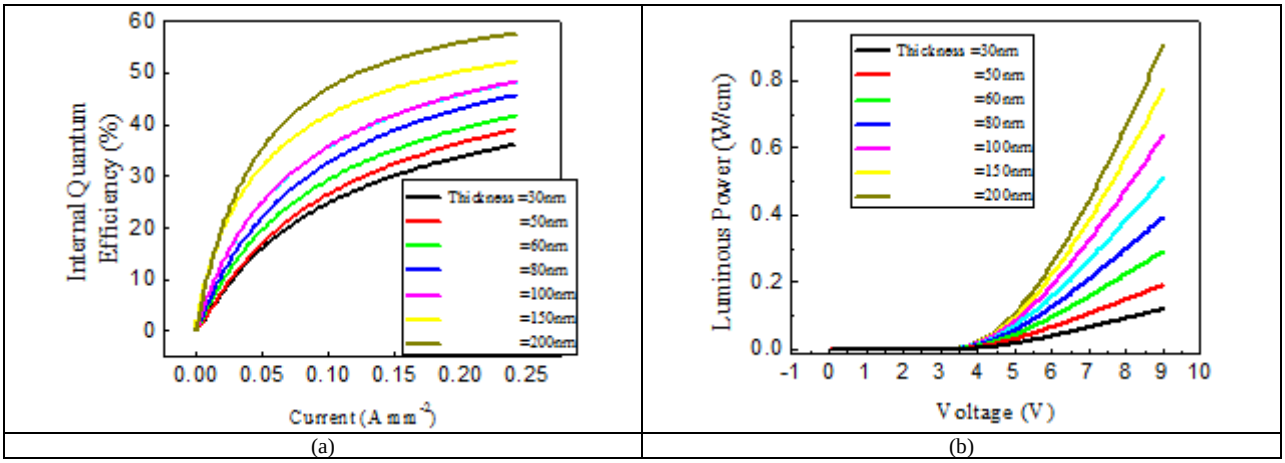
ACTIVE REGION

In the simulation, we have implemented $Cd_{0.15}Zn_{0.85}O$ as the heterostructure LED active region. The active region is sandwiched between a top p-type $Mg_xZn_{1-x}O$ electron barrier layer and a bottom n-type $Mg_xZn_{1-x}O$ hole barrier layer. The simulated emission spectra for heterostructure LED as a function of active layer parameters at room temperature are shown in Fig.8. The radiative emission band with a peak at 430 nm originates from the near- band transition in the $Cd_{0.15}Zn_{0.85}O$ active region. When thickness is increased from 30 nm to 200 nm, carriers effectively confine in the active region which increases the probability of radiative recombination under forward bias and five times increment in emission intensity is observed. The threshold voltage also improves from 3.6V to 3.3V when the thickness is varied.



(a) (b)

Fig.8 Simulated (a) emission spectra and (b) I-V characteristics for the active layer ($Cd_{0.15}Zn_{0.85}O$) thickness of heterostructure LED



(a) (b)

Fig.9 Simulated (a) internal quantum efficiency and (b) luminous power for the active layer ($Cd_{0.15}Zn_{0.85}O$) thickness of heterostructure LED

In Fig.9, as the thickness of active region is increased, there will be additional confinement of charge carriers which increases the internal quantum efficiency from 30% to 55%. The luminous power increases from 0.1 W to 0.7 W as the thickness is increased from 30 nm to 200 nm due to enhanced recombination rate in the active region. The other parameters of heterostructure LED are kept constant when layer thickness is increased.

TOP CONTACT LAYER

The p-ZnO layer has been taken as a top contact layer for heterostructure LED device. Here we have considered doping concentration and layer thickness parameter variation for the device structure.

Concentration

The EL intensity and threshold voltage increases on increasing the dopant concentration from 5×10^{16} to 5×10^{18} cm^{-3}. As more holes are available for recombination with electrons thus carrier injection rate increases [13]. The thickness is kept constant at 50 nm when doping concentration is altered from 5×10^{16} cm^{-3} to 5×10^{18} cm^{-3} .

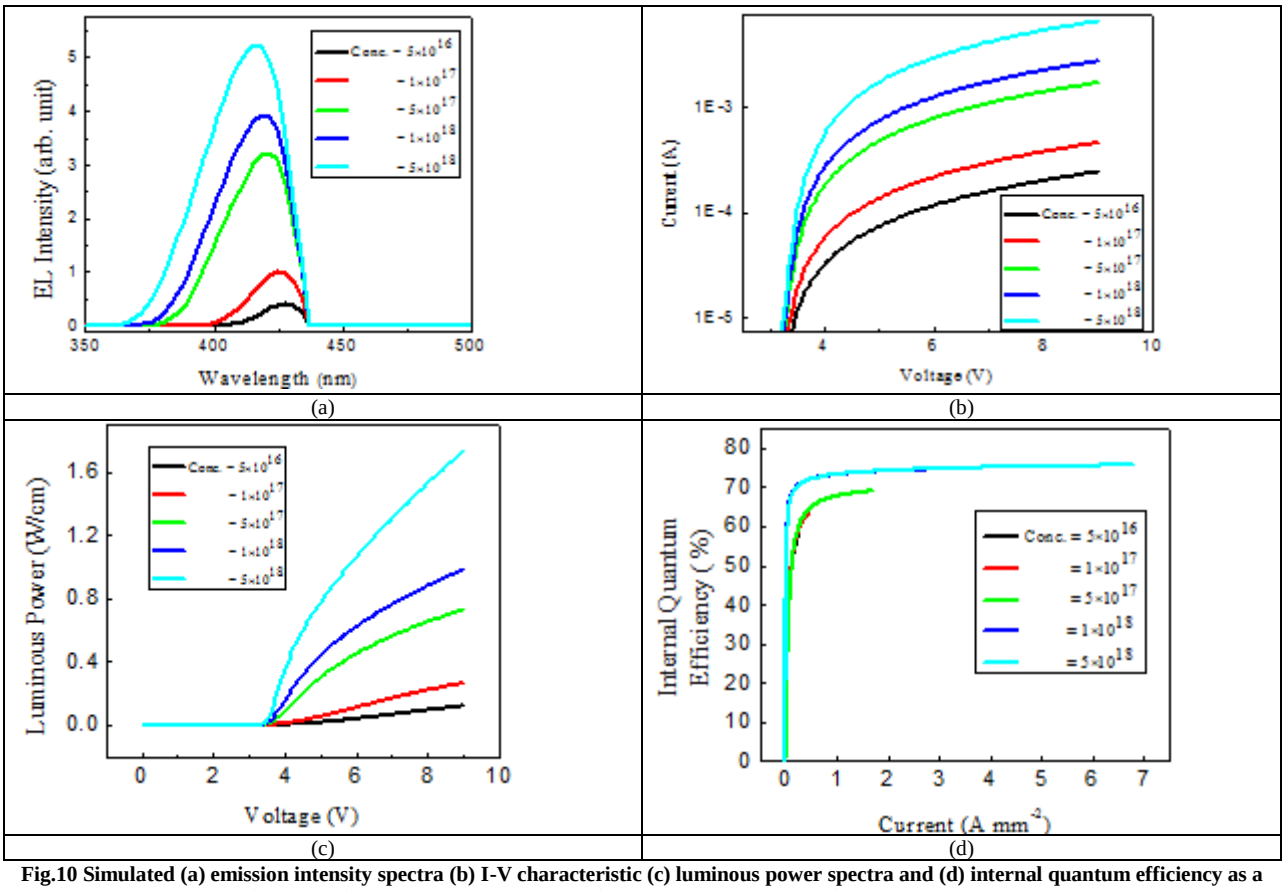
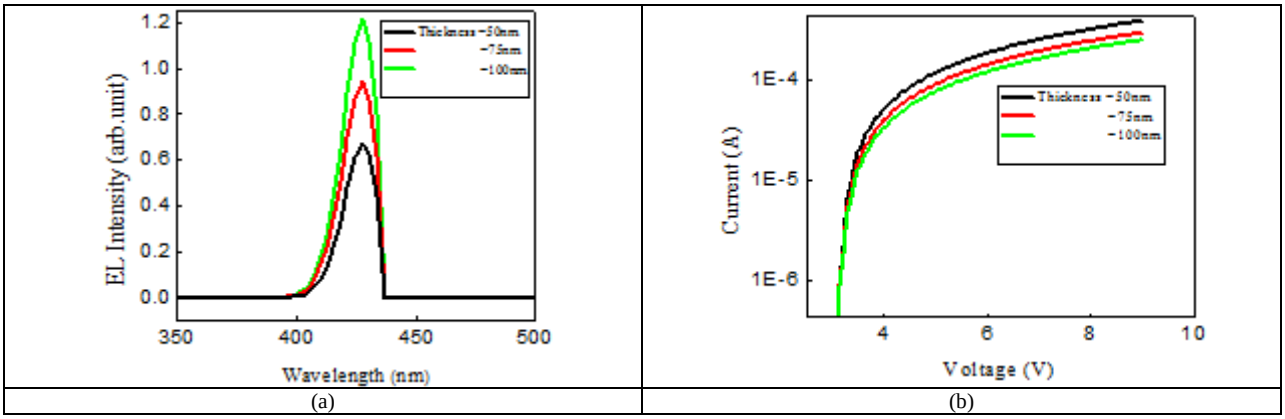
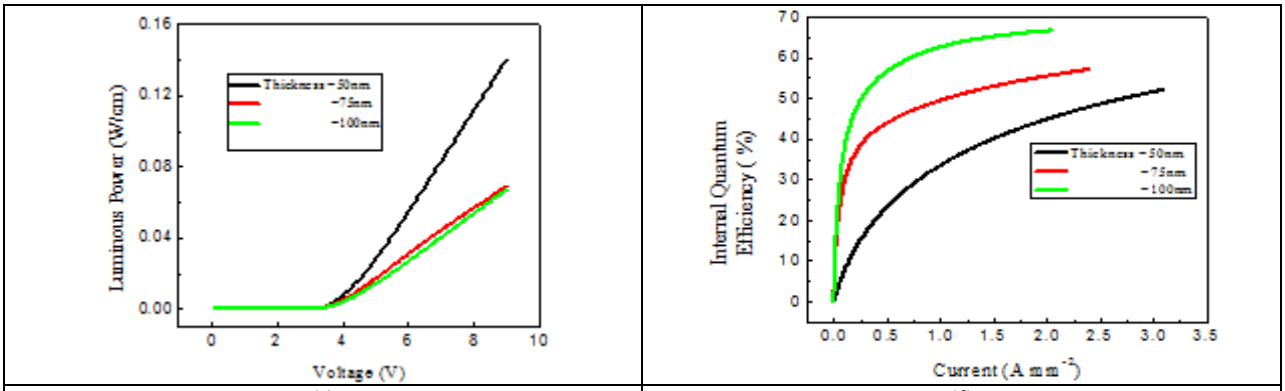


Fig.10 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of hole doping concentration for the top contact layer of heterostructure LED





(c) (d)

Fig.11 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of layer thickness for the top contact layer of heterostructure LED

Thickness

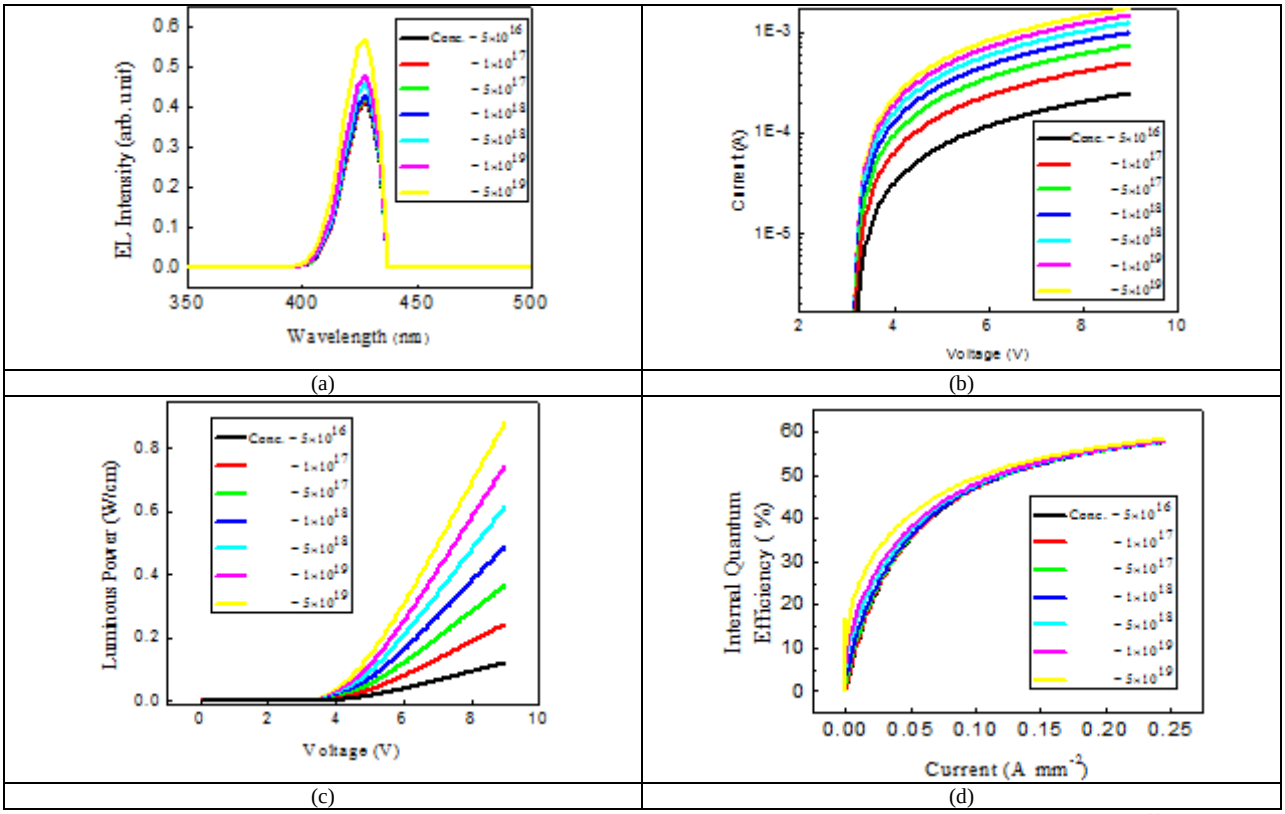
As seen from Fig.11, the emission intensity increases while threshold voltage and power decreases on increasing the thickness from 50 nm to 100 nm. Since increases in thickness results in lowering of valance band barrier for hole injection thus there will be significant increase in quantum efficiency. On increasing thickness, the doping solubility decreases strong defect related emission arises for p-ZnO layer. During thickness variation doping concentration is fixed at 5×10^{16} cm^{-3}.

BOTTOM CONTACT LAYER

The n-ZnO layer has been taken as a bottom contact layer for heterostructure LED device. Here we have considered doping concentration and layer thickness parameter variation for the device structure.

Concentration

As mentioned in Fig.12, the emission intensity increases on increasing the doping concentration from 5×10^{16} to 5×10^{19} cm^{-3}. The threshold voltage characteristic shows only a slight variation from 3.2V to 3.4V while luminous power increases from 0.1 W to 0.8 W for higher doping concentration. At this point it is noted that thickness is held constant at 50 nm.



(a) (b)

(c) (d)

Fig.12 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of electron doping concentration for the bottom contact layer of heterostructure LED

Thickness

The EL peak emission in Fig.13 is attributed to radiative electron-hole recombination in ZnO layer, due to large conduction band offset. As the thickness of ZnO layer is increased from 50 nm to 500 nm, the carriers capture probability shows a fourfold increment. The doping concentration is kept constant at 5×10^{16} cm^{-3} when the thickness is varied.

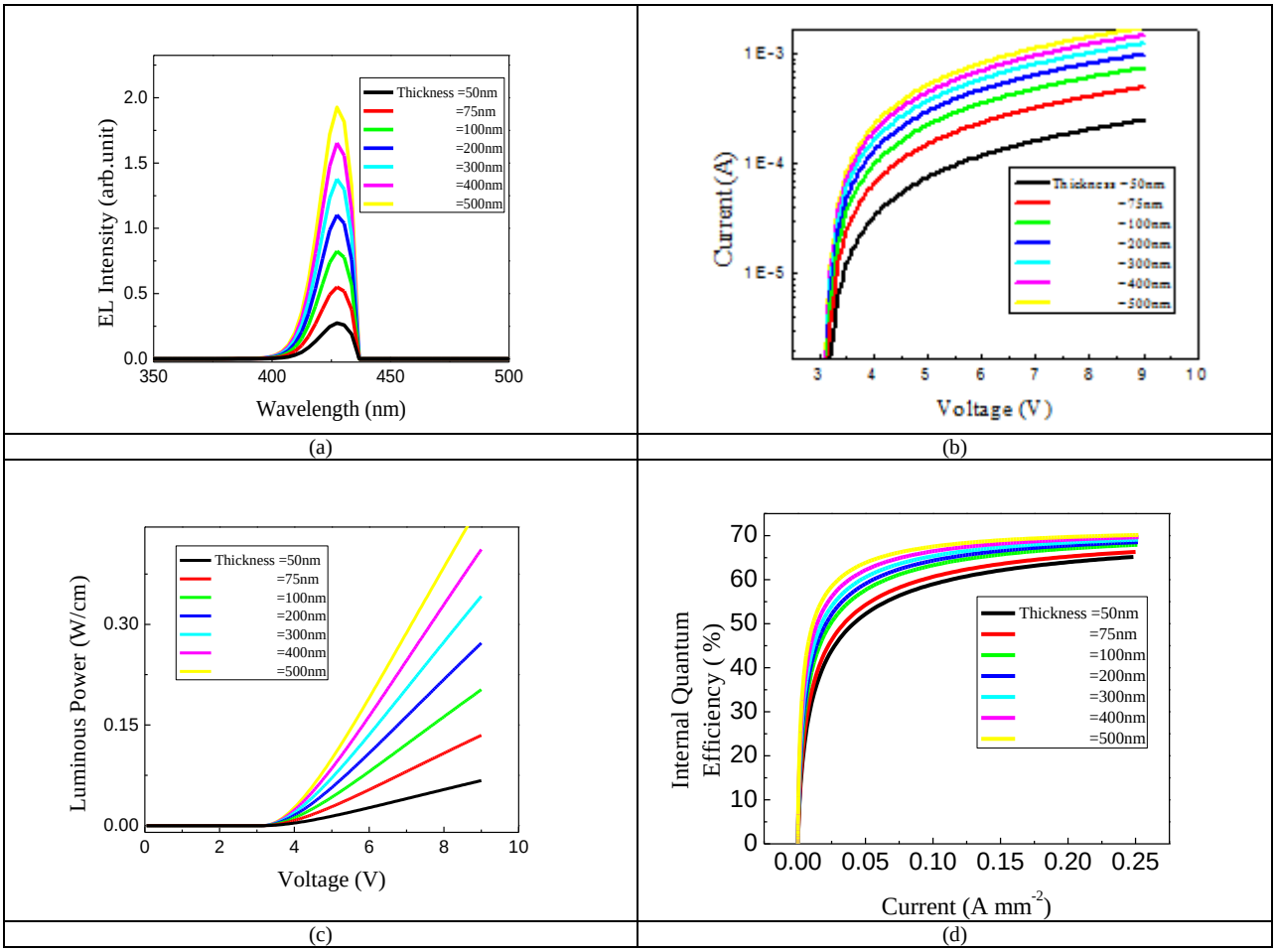


Fig.13 Simulated (a) emission intensity spectra (b) I-V characteristic (c) luminous power spectra and (d) internal quantum efficiency as a function of layer thickness for the bottom contact layer of heterostructure LED

CONCLUSION

We present detailed theoretical investigation of optimized device structure of MgZnO/CdZnO/MgZnO based double heterostructure bluish LED. The LED emits at 430 nm with an IQE value of ~70% at an anode current of 0.22A at room temperature. Factors largely affecting the device internal quantum efficiency of double heterostructure LED; including doping concentration, thickness of active and barrier regions; are numerically examined in detail. Our work identified several key aspects for developing high quality zinc oxide films and heterostructure design for device applications. The results shows the potential of ZnO-based material for optical and quantum electronics applications. Due to its increased lifetime, reduced power consumption and brightness, Blue light emitters are preferred for displays, scanners, data storage, street lightings and traffic signals. The double heterostructure approach provides an alternative for achieving robust *p*-type doping for ZnO-based LED that incorporates CdZnO active regions with optimized composition and thickness.

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