Theoretical Investigation of MgZnO/CdZnO/MgZnO Double Heterostructure Bluish LED with Improved Internal Quantum Efficiency

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***Abstract*—A design approach for zinc oxide (ZnO) based double heterostructure light emitting diode (LED) has been proposed to achieve near band edge bluish electroluminescence around 430 nm with internal quantum efficiency (IQE) of 55%. Rigorous theoretical investigation has been performed for the device 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.**

***Index Terms*—double heterostructure, quantum efficiency, bluish zno led, electroluminescence**

I. 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 costs 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 can be increased up to 4.0 eV by incorporating Mg in the ZnO layer while still maintaining the wurtzite structure [3], [4]. Similarly, Cd incorporation in ZnO results in the reduction of band gap energy since CdO (2.3 eV) has smaller band gap [5]. There are several reports [6], [7], [8] on the growth of heterostructure materials to form LEDs; however, in all those cases, the hetero-interfaces have 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 [8].

Here we adopted all ZnO layers approach on silicon substrate. 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. Several parameters have been considered for 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 [9]. 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) [10]. 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.

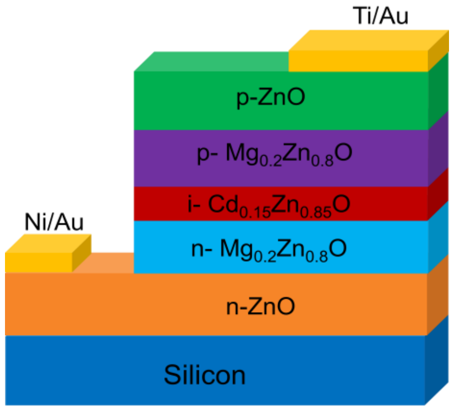

Figure 1. Cross sectional view of the heterostructure LED.

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Fig. 1 presents the cross-sectional view of the device studied in this paper. In this paper, a comprehensive report regarding design parameters for the ZnO-based heterostructure

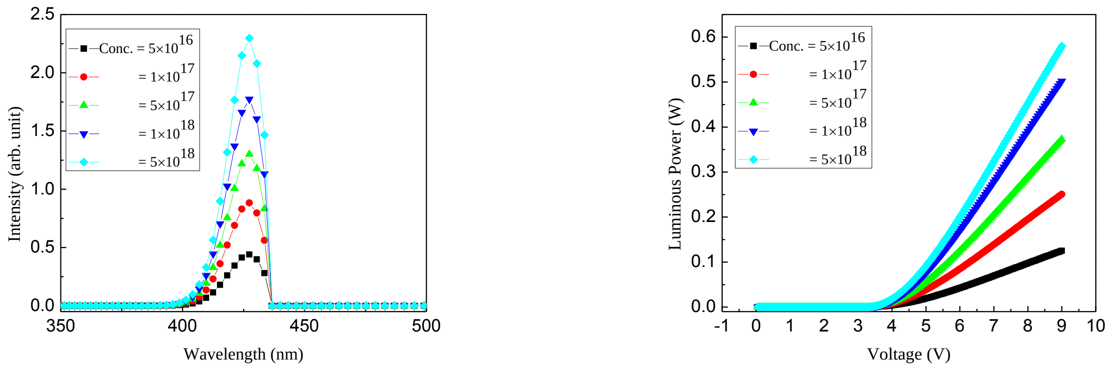
LED in terms of constituent layer structure, doping and composition and their effect on light emission from the device and its threshold behavior is thoroughly examined.

II. Device Structure

This section describes the device structure, with the layer characteristics for IQE optimization. On top of the substrate, an n-type ZnO buffer layer is deposited and this layer behaves as a cap layer to prevent the escaping of electrons. The effect of thickness and doping concentration of buffer layer on the device performance has been investigated. An n-type MgZnO layer is grown on the top of cap layer which will act as a barrier for holes. The effect of barrier thickness, doping concentration, and composition, on the behavior of the device has been studied using device simulation software [11]. In the heterostructure device, the $Cd_{0.15}Zn_{0.85}O$ layer is considered to be the active region. On top of the active region, an electron blocking layer of MgZnO is deposited and this layer will act as a current spreading layer. 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 p-type ZnO cap layer. Au/Ni and Au/Ti were taken as electrodes to make good ohmic contacts [12]. In the simulation the device width is considered to be 1 µm and band edge emission at room temperature is calculated at a forward bias potential of 7 V.

A. *Electron Blocking Layer (EBL)*

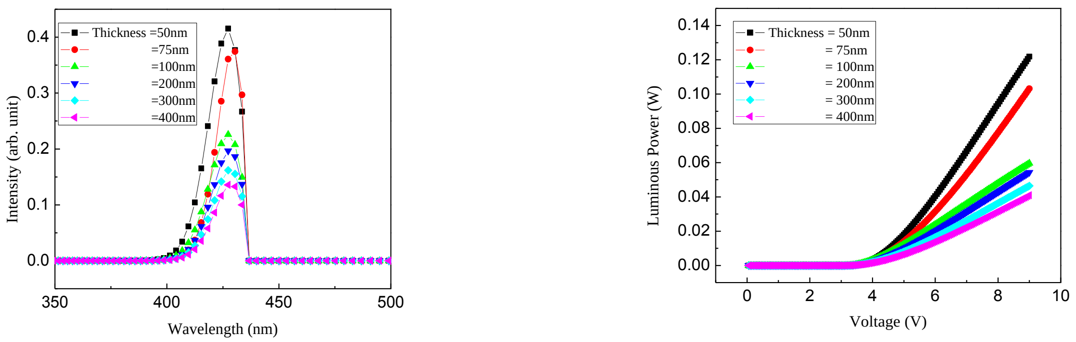
In the heterostructure LED, p-type $Mg_{0.2}Zn_{0.8}O$ acts as the electron blocking layer. This layer acts as a barrier to prevent electrons to escape from the $Cd_{0.15}Zn_{0.85}O$ active region. Fig.2 represents the intensity and luminous power spectra of the device structure with respect to hole doping concentration of the EBL. It is to be noted that the thickness of the EBL layer is held constant at 50 nm when its doping concentration is varied



(a) (b)

Figure 2. Simulated (a) emission spectra and (b) power spectra of heterostructure LED as a function of hole doping concentration of the EBL layer.

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 doping concentration (from 5×10^{16} to 5×10^{18}) cm^{-3}.As we increase the doping concentration, there is a significant increase in emission intensity from 0.5 to 2.25 W/(cm^2 µm) due to effective carrier confinement. The threshold voltage also improves from 3.6V to 3.3V and an increase in luminous power is observed under the same bias voltage for higher carrier density.



(a) (b)

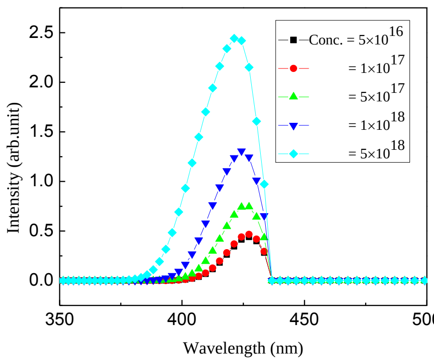
Figure 3. Simulated (a) emission spectra and (b) power spectra of heterostructure LED as a function of EBL thickness

Fig. 3 shows the intensity and power spectra variation with respect to EBL layer thickness. As the thickness is increased from 50 nm to 400 nm, the electroluminescence decreases from 0.42 to 0.13 W/(cm^2 µm). The current voltage characteristics demonstrate increased device series resistance with the increase in thickness and this is illustrated by the increase of threshold voltage from 3.4 V to 3.6 V when EBL layer thickness is increased from 50 nm to 400 nm. The doping concentration is fixed at 5×10^{16} when the thickness of EBL is varied.

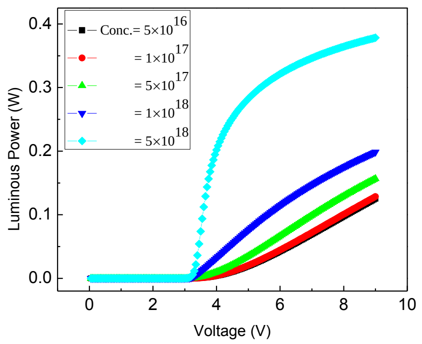
B. Hole Blocking Layer (HBL)

Similar to the EBL optimization, the optimization of the hole blocking 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.

It is seen from Fig.4 (a) that as the electron doping concentration is increased, of the HBL layer is increased from 50 nm to 400 nm, a four-fold increment of electroluminescence intensity is observed. At this point, it should be noted that the thickness of the HBL layer is held constant at 50 nm when its doping concentration is altered.



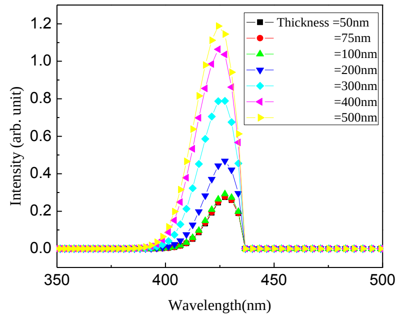
(a)



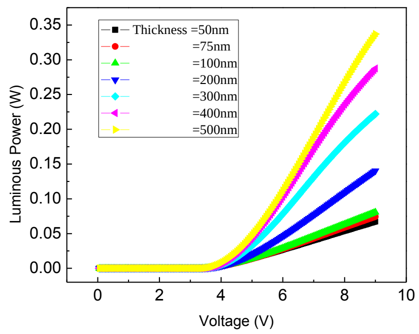
(b)

Figure 4. Simulated (a) emission spectra and (b) power spectra of the heterostructure LED as a function of electron concentration of the HBL layer.

From Fig.5, 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, a reduction in the device threshold voltage (from 3.3V to 3.6V), as is illustrated in Fig.5 (b), is noticed for the corresponding increase in the HBL thickness. The doping concentration is fixed at 5×10^{16} cm^{-3} when the thickness of HBL is varied. 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. region.

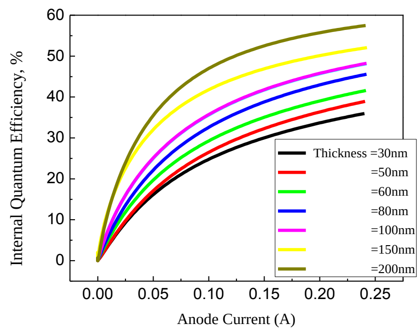


(a)

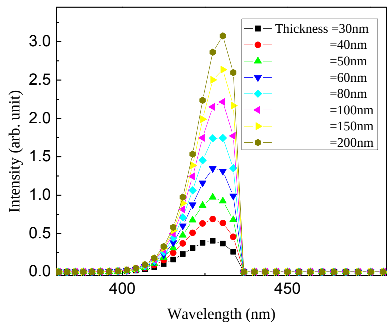


(b)

Figure 5. Simulated (a) emission spectra and (b) power spectra of the heterostructure LED as a function of HBL thickness.



(a)



(b)

Figure 6. Simulated (a) internal quantum efficiency and (b) emission spectra from the heterostructure LED for different thicknesses of Cd0.15Zn0.85O active layer.

C. 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 $Mg_{0.2}Zn_{0.8}O$ electron blocking layer and a bottom n-type $Mg_{0.2}Zn_{0.8}O$ hole blocking layer. It can be seen from fig.6 (a). 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%. Similarly from fig. 6 (b), 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 significant increase in emission intensity from 0.5 to 2.25 W/(cm^2 μm) is observed.

III. Conclusion

In conclusion, we have theoretically demonstrated near band edge bluish electroluminescence around 430 nm with an IQE value of 55% from the ZnO material system based double heterostructure LED. 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.

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