Numerical Simulation of ZnO-based LEDs

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***Abstract*—Optimizing the internal quantum efficiency (IQE) is very important for UV LEDs, since the present generation of devices has very low IQE. This is particularly important for ZnO-based LEDs that are still technologically immature. This work presents the preliminary results of an ongoing investigation intended to identify the optimization criteria for the design of ZnO-based LEDs.**

I. Introduction

Zinc oxide and its ternary alloys have become increasingly interesting for the design and fabrication of UV-LEDs due to potential advantages over III-V nitrides, such as substrate availability, comparatively simpler growth and processing technologies, and larger exciton binding energy. The large energy gap of ZnO (3.373 eV) and the bang-gap engineering possibilities offered by CdZnO, for narrower gap, and (Mg,Be)ZnO, for wider gap, makes them very interesting for the realization of LEDs in the green, blue and near ultraviolet spectral regions. Because of their characteristics, these ternary alloys are increasingly being employed as possible materials for the construction of multi-quantum-well devices. Unfortunately, there are still significant difficulties in achieving reliable p doping [1]. Furthermore, high spontaneous and piezoelectric charges at interfaces between layers make the device design and optimization difficult [2]. Ultimately, the presence of these charges degrades the internal quantum efficiency of the device. Therefore it is important to establish a set of design criteria for ZnO-based LEDs that may lead to device structures with high internal quantum efficiency (IQE). Our device analysis has been based on a two-dimensional drift-diffusion model coupled with several quantum corrections, including the self-consistent solution of Poisson and Schrödinger equations. The modelling approach and the specific material parameters for ZnO have been presented in [3] and [4], respectively.

The goal of the present work is to perform a preliminary investigation to understand which are the most important design parameters that need to be optimized to obtain LEDs with high IQE. Specifically we will consider the effect of the geometrical and the doping characteristics of the layers included in the device and the effect of the interface charges due to spontaneous and piezoelectric polarization.

II. Simulations Results

Fig. 1 presents the cross section of the device structure analyzed in this work. Several parameters need to be considered when studying the performance of this device structure. Following the methodology outlined in [3] we consider both the geometrical, composition and doping characteristics of each layer in the device of Fig. 1.

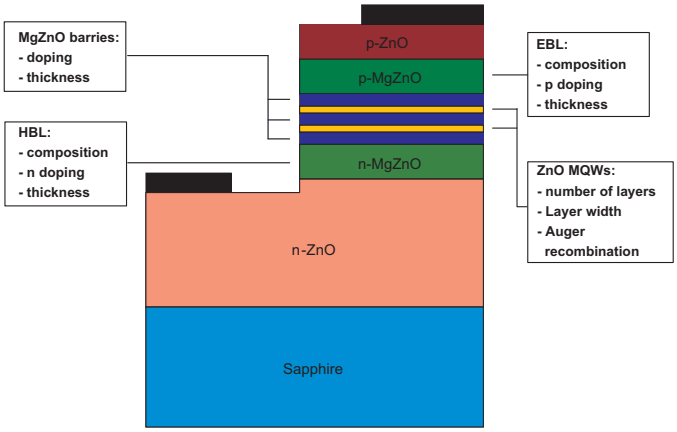

Fig. 1. ZnO-based LED device structure analyzed in this work.

As an example, we consider a structure with an active region with three ZnO quantum wells (QWs) separated by $Mg_{0.1}Zn_{0.9}O$ barrier layers, surrounded by a $Mg_{0.2}Zn_{0.8}O$ electron blocking layer (EBL) and a $Mg_{0.1}Zn_{0.9}O$ hole blocking layer (HBL). The barriers and wells are undoped, the EBL is supposed to be lightly p-doped with $10^{16}\,\mathrm{cm}^{-3}$ acceptors, and the hole concentration of the ZnO p-type cap is supposed to be $7\cdot10^{16}\,\mathrm{cm}^{-3}$. The device is 200$\mu$m wide and it is grown on a 1 μm thick ZnO buffer layer n-doped with $5\cdot10^{19}\,\mathrm{cm}^{-3}$ donors.

For each one of these layers one needs to determine an appropriate doping, molar concentration and thickness to achieve the highest possible IQE. Furthermore, one needs also to take into account several technological limiting factors, for example the limited p-type doping level for ZnO and MgZnO layers.

As an example, the inset of Fig. 2 presents the calculated IQE as a function of the forward bias current for different compositions of the EBL. It can be seen that the IQE is in general quite low, reaching 3 % only at high forward current. Furthermore, changing the EBL composition does not significantly impact the IQE. The reason behind this low IQE can be traced back to the effect of the polarization charges that lead to a poor overlap between electron and holes wavefunctions in the QWs. These are shown in Fig. 3. It can be immediately noticed that, as a result of the spontaneous and piezoelectric polarization, the resulting tilt in the conduction and valence band profiles leads to an almost complete decoupling of the two sets of electrons and holes wavefunctions.

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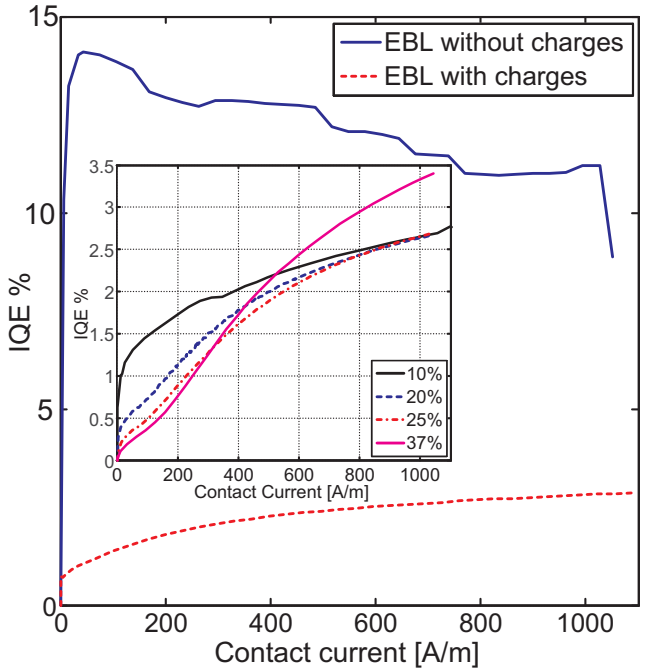

Fig. 2. *Main figure*: Calculated IQE for the same ZnO/MgZnO LED structure with and without polarization charges at the interface between barrier and EBL layers. *Inset*: Calculated IQE as a function of the forward current for different compositions of the EBL.

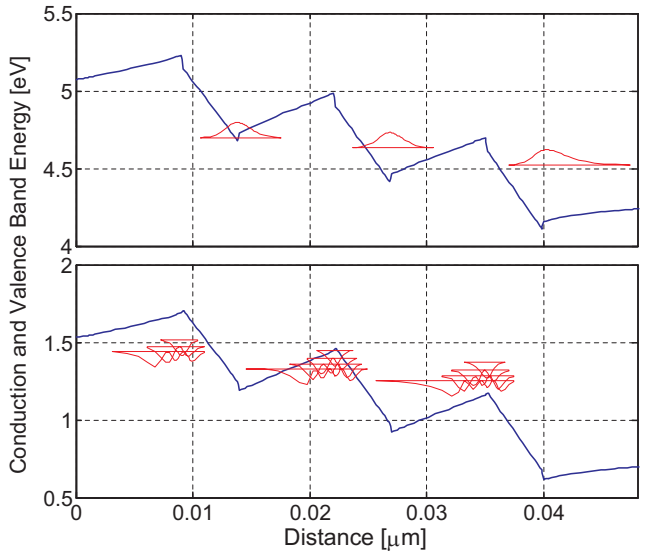

Fig. 3. Calculated electron and hole wavefunctions.

A possible strategy to mitigate this problem would be to use narrow QWs in order to reduce the effect of the polarization fields. In general, for ZnO this approach is not as effective as it is for GaN, since the polarization charges are larger for a given confinement in the QW. Fig.4 presents the calculated IQE for a GaN-based LED having the same emission wavelength and QW confinement. It can be seen that the IQE is significantly higher in the GaN-based LED than in the ZnO-based one. To understand this result one has to look at the magnitude of the

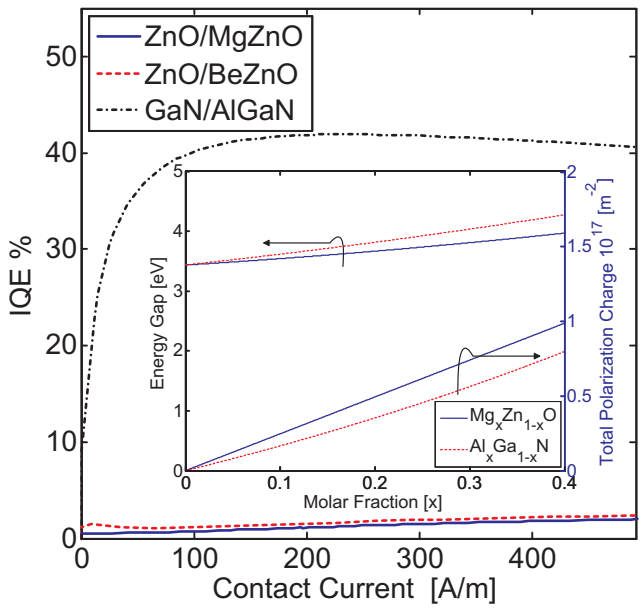

Fig. 4. *Main figure*: Calculated IQE for a GaN/AlGaN LED (dashed-dot line), a ZnO/MgZnO based LED (solid line) and a ZnO/BeZnO based LED (solid line) having the same geometry and band offset. *Inset*: Calculated energy gap and polarization charges for AlGaN and MgZnO layers.

polarization charges. The inset of Fig. 4 presents the energy gap and the polarization charges for AlGaN and MgZnO, computed assuming GaN and ZnO wells respectively, as a function of the molar fraction. It can be observed that, to obtain the same band offset in a ZnO/MgZnO and a GaN/AlGaN heterojunction, the Mg content of the MgZnO layer must be higher than the Al molar fraction of the AlGaN barrier. This leads to a larger crystal mismatch resulting in a significantly larger polarization field. Finally, we can note that a BeZnO barrier would require a lower Be molar fraction, but would not provide any improvement since the total polarization charge at the heterointerface would be about the same as in the ZnO/MgZnO structure.

Acknowledgment

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