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

![Fig. 1. ZnO-based LED device structure analyzed in this work.](image-url)
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 polarization charges. The inset of Fig. 4 presents the energy gap and the polarization charges for AlGaN and MgZnO layers.

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REFERENCES


