Published in: Appl. Phys. Lett. **87**, No. 24, 243502 (2005) / DOI 10.1063/1.2140873

Simulation of hybrid ZnO/AlGaN single-heterostructure light-emitting diode

K. A. Bulashevich[1], I. Yu. Evstratov[1], V. N. Nabokov[1], and S. Yu. Karpov[*1,2]

[1] Soft-Impact, Ltd., P.O.Box 83, 27 Engels av., St.Petersburg, 194156 Russia
[2] Semiconductor Technology Research, Inc., P.O.Box 70604, Richmond, VA, 23255-0604, USA

Received 20 June 2005, accepted 13 October 2005
Published online 5 December 2005

PACS 85.60.Jb, 85.30.De, 78.30.Fs, 77.65.Ly

Using simulations, we have examined specific features of a hybrid n-ZnO/p-AlGaN light-emitting diode (LED) operation, originated from a type-II band alignment and a negative polarization charge at the ZnO/AlGaN interface. These factors are found to improve the carrier confinement near the interface and to affect significantly the light emission spectra and internal quantum efficiency of the LED. The theoretical predictions are compared with available observations.

Preprint (2005)

Zinc oxide is a wurtzite semiconductor with a direct bandgap of ~3.37 eV at room temperature and a high exciton binding energy of ~60 meV that further increases in a quantum well [1]. Being doped with impurities, ZnO is capable of providing both electron and hole conductivity. These properties as well as the commercial availability of native substrates make ZnO and MgZnO alloys very promising materials for fabrication of high-efficiency UV LEDs and laser diodes. While ZnO serves as an active layer, MgZnO can be used for carrier confinement in an LED heterostructure due to a wider bandgap. However, among binary ZnO, CdO, and MgO compounds, zinc oxide is the only semiconductor with thermodynamically stable wurtzite phase. This limits, in particular, the allowable range of wurtzite $Zn_{1-x}Mg_xO$ composition variation by the value of $x \approx 0.15$ [2] and, hence, the available conduction and valence band offsets. In addition, a sufficiently high p-doping of group-II oxides necessary for device fabrication is not yet reliably obtained. All this has stimulated investigations of hybrid ZnO/AlGaN LEDs providing an alternative solution of the above problems.

The modelling reported in this paper is aimed at a better understanding of the operation of MQW LED heterostructures with the focus on the carrier confinement in the active region and the role of selective doping in the barriers separating individual quantum wells. This research was stimulated by the reported improvement of the LED efficiency and wavelength stability due to enhanced barrier doping [4,6].

A ZnO/AlGaN heterojunction exhibits a type-II band alignment [3] and a small, ~1.8-4.0% , lattice mismatch between the contacting materials. The latter enables one to expect a reduced density of surface traps at the ZnO/AlGaN interface, giving rise to non-radiative carrier recombination. Recently a single-heterostructure (SHS) ZnO/AlGaN and a triple-heterostructure (THS) MgZnO/ZnO/AlGaN/GaN LEDs operating in the spectral range of 370-410 nm have been demonstrated in [4,5]. These studies have given basic ideas of hybrid-LED structure design and provided the data on the device characteristics. However, specific features of the carrier injection and light emission originated from the type-II band alignment and the effect of the interface polarization charge on the LED band diagram still remain obscure. In this paper, we report on modeling analysis of a ZnO/AlGaN hybrid LED that demonstrates (i) efficient

[*] Corresponding author: e-mail: karpov@semitech.us

carrier confinement in the SHS due to a polarization charge at the ZnO/AlGaN interface and (ii) specific mechanism of tunnel radiative recombination near the heterojunction.

In order to highlight the specificity of hybrid ZnO/AlGaN LEDs, we focus on the simplest SHS suggested in [4]. It consists of a p-$Al_{0.12}Ga_{0.88}N$ layer 0.8 μm thick grown on an n-GaN buffer layer, followed by 1.0 μm n-ZnO. The electron and hole concentrations in n-ZnO and p-AlGaN are of 7×10^{17} cm^{-3} and 5×10^{17} cm^{-3}, respectively. Simulation of the LED operation has been performed with the SiLENSe 2.0 package [6] based on the drift-diffusion approach to the carrier transport. The model accounts for both radiative and non-radiative electron and hole recombination on threading dislocations [7], polarization charges at the structure interfaces, and the complex valence band structure of wurtzite semiconductors in terms of the 8×8 Kane Hamiltonian [8]. The physical properties of III-nitrides chosen for the simulation are close to those recommended in the review [9]. The properties of ZnO are borrowed from [5].

The LED structure is considered as grown in the [0001] direction, i.e. the crystal is assumed to have a metal polarity that controls a negative polarization charge at the ZnO/AlGaN interface. Accounting for the thickness of the p-AlGaN layer, we assume it to be completely relaxed with respect to the underlying GaN buffer layer, while the ZnO layer is considered to be coherently grown on AlGaN and, hence, strained. The threading dislocation density of 10^9 cm^{-2}, typical of III-nitride epitaxial materials grown by metalorganic chemical vapor deposition, is chosen for the simulation.

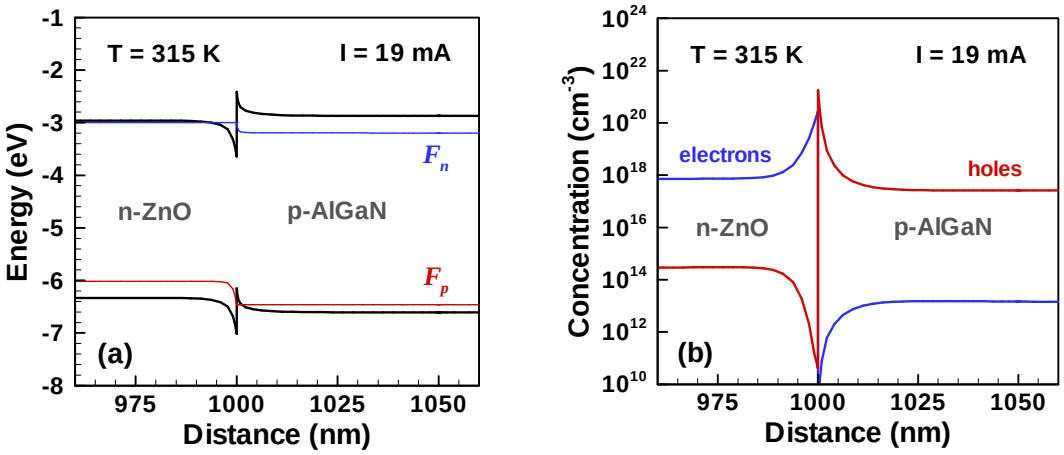

Fig. 1 Band diagram (a) and distributions of carrier concentrations (b) of the hybrid ZnO/AlGaN SHS LED from Ref.[4].

Fig.1a shows the band diagram of the hybrid SHS LED computed for 315 K and the forward bias providing the electric current of ~20 mA at the contact area of 0.04 cm^2. Due to the negative polarization charge induced at the ZnO/AlGaN interface and the type-II band alignment, local quantum wells for both electrons and holes are formed next to the heterojunction. This results in a considerable increase of the electron and hole concentrations near the interface (Fig.1b), providing an effective carrier confinement that is not typical of conventional SHSs. This effect is predicted to occur at a certain bias ~2.6 V which is a function of the doping level. At a lower bias, the electronic quantum well disappears, and the electron concentration at the interface falls down dramatically. In contrast, the hole quantum well exists in the whole range of forward bias variation, which is due to the negative interface polarization charge attracting holes.

The I-V characteristic of the hybrid LED computed for 350 K and the diode series resistance of 12 Ω fits well the experimental curve (Fig.2a). The predicted temperature shift of the turn-on voltage correlates well with the data on THS hybrid LED reported in [5]. Fig.2b plots the internal quantum efficiency (IQE) of the SHS LED as a function of current density computed for different operation temperatures. It is interesting that the IQE at 300K falls down below the IQE computed for 500 K as

soon as the current density becomes greater than ~0.4 A/cm^2. For the IQE at 315 K, however, this occurs already at ~ 0.8 A/cm^2. We have also found that the ratio of the IQEs predicted for 315 K and 500 K correlates well with the ratio of the integral electroluminescence intensities measured at 300 K and 500 K at the electric current of 20 mA [4].

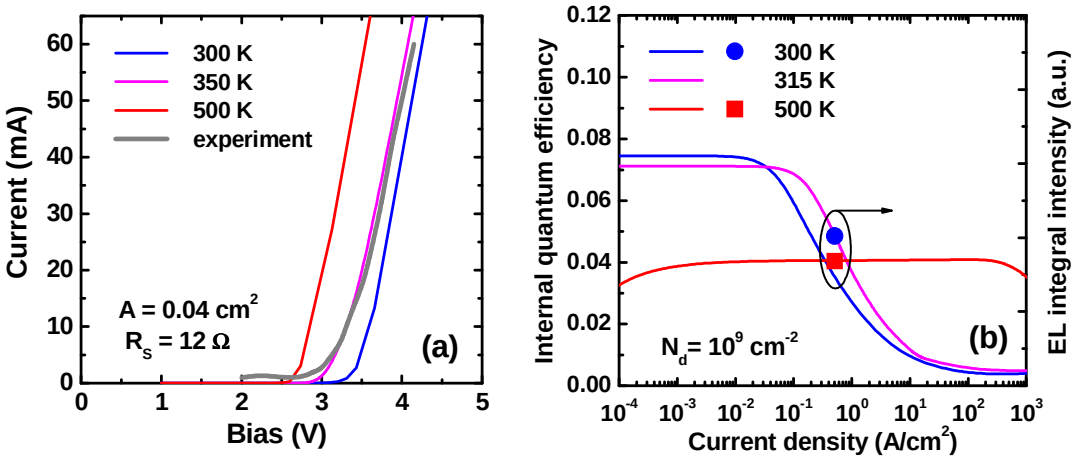

Fig. 2 I-V characteristic (a) and internal quantum efficiency as a function of current density (b) of the ZnO/AlGaN LED computed for different temperatures.

It should be noted that the current-density dependence of IQE shown in Fig.2b is qualitatively different from that computed for conventional InGaN/AlGaN LEDs where the IQE rises with current due to saturation of the non-radiative recombination channel (see, e.g. [10]). Our computations show that the IQE fall down predicted for high current densities and temperatures of 300-350 K is caused by the enhanced electron penetration into p-AlGaN where a considerable part of the minority carriers recombine non-radiatively on threading dislocations. Due to modification of the band diagram, this effect is much less pronounced at 500 K. In order to suppress the undesirable minority carrier penetration, an electron blocking layer inserted into the p-AlGaN emitter might be helpful.

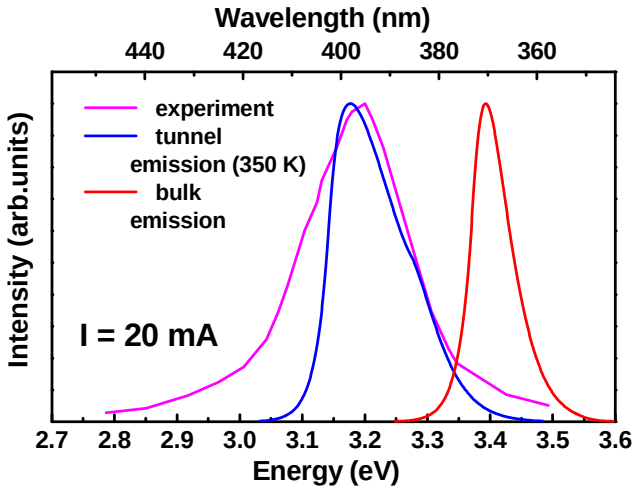

Fig. 3 Light emission spectra originated from the tunnel electron-hole recombination and from bulk ZnO compared with the spectrum measured in [4].

The appearance of the adjacent electron and hole quantum wells at the ZnO/AlGaN interface makes possible a tunnel radiative recombination of the carriers confined in the wells. Fig.3 compares the

emission spectrum from the bulk ZnO (dash-dotted line) and that computed with account of tunnel recombination only (solid line) with the spectrum reported in [4] and attributed to 300 K. In the computations, a uniform spectrum broadening of 20 meV has been assumed. It is seen that the predicted peak position and the short-wavelength wing of the tunnel-emission spectrum correlates well with the data of [4]. The more extended long-wavelength wing of the experimental spectrum may be explained by a contribution of defects in ZnO and a non-uniformity of the ZnO/AlGaN heterojunction but, in any case, it needs more efforts to be completely understood.

The comparison of the theoretical predictions with observation given in Figs.2-3 shows that the modeling approach used in our study is capable of reproducing the principal features of hybrid LEDs, if an uncertainty in the operation temperature from 300 to 350 K is allowed. This uncertainty may be associated with a possible overheating of the LED active region, which was not discussed in [4], a strain relaxation in ZnO, as well as with the poorly know polarization properties of ZnO and insufficient information on the ZnO/AlGaN interface microstructure (first of all, abruptness and surface traps availability).

In conclusion, we have analyzed specific features of hybrid ZnO/AlGaN LED operation in terms of modeling. In the SHS LED structure considered in the paper, the type-II band alignment in combination with a negative polarization charge at the heterojunction is found to result in a pronounced tunnel radiative recombination near the ZnO/AlGaN interface and an IQE that degrades at a high current through the diode. The theoretical predictions fit quite reasonably the available observations. Further progress in understanding of the hybrid LED operation requires, in our opinion, to refine the ZnO materials parameters and to get more experimental information on the nature of the ZnO/AlGaN interface, including availability and properties of surface traps.

References

[1] T. Makino, Y. Segawa, M. Kawasaki, and H. Koinuma, Semicond. Sci. Technol. **20**, S78 (2005).
[2] A. Ohmoto and A. Tsukazaki, Semicond. Sci. Technol. **20**, S1 (2005).
[3] S.-K. Hong, T. Hanada, H. Makino, Y. Chen, H.-J. Ko, T. Yao, A. Tanaka, H. Sasaki, and S. Sato, Appl. Phys. Lett. **78**, 3349 (2001).
[4] Ya. I. Alivov, E. V. Kalinina, A. E. Cherenkov, D. C. Look, B. M. Ataev, A. K. Omaev, M. V. Chukichev, and D. M. Bagnall, Appl. Phys. Lett. **83**, 4719 (2003).
[5] A. Osinsky, J. W. Dong, M. Z. Kauser, B. Hertog, A. M. Dabiran, C. Plaut, P. P. Chow, S. J. Pearton, X. Y. Dong, and C. J. Palmstrom, Electrochem. Soc. Proceedings **2004-6**, 70 (2004).
[6] http://www.semitech.us/products/SiLENSe/
[7] S. Yu. Karpov and Yu. N. Makarov, Appl. Phys. Lett. **81**, 4721 (2002).
[8] S. L. Chuang and C. S. Chang, Phys. Rev. B **54**, 2491 (1996).
[9] I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).
[10] S. Yu. Karpov, K. A. Bulashevich, I. A. Zhmakin, M. O. Nestoklon, V. F. Mymrin, and Yu. N. Makarov, Phys. Status Solidi B **241**, 2668 (2004).