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Ultra-violet light-emitting diodes with quasi acceptor-free AlGaN polarization doping

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Abstract The development and application of nitride-based light-emitting diodes (LEDs) is handicapped by the low hole conductivity of Mg-doped layers. Mg-doping becomes increasingly difficult with higher Al-content of the p-AlGaN layers as required for ultra-violet (UV) light emission. Polarization-induced hole doping of graded AlGaN was recently demonstrated as an alternative doping method. Using advanced numerical device simulation, this paper investigates the impact of polarization-doping on the internal device physics of UV-LEDs and compares the conventional Ga-face growth to the novel N-face growth direction. Various LED design options are explored to maximize the internal quantum efficiency.

Keywords Light-emitting diode · LED · Ultra-violet · AlGaN · Doping · Grading · Acceptor · Polarization · Internal quantum efficiency

1 Introduction

GaN-based light-emitting diodes (LEDs) are currently of great interest for applications in lighting, displays, sensing, biotechnology, medical instrumentation and other areas. However, the development of nitride-based LEDs is handicapped by the low electrical conductivity of p-doped material. Heavy Mg doping is required to achieve a sufficient density of free holes, which lowers the hole mobility. Mg-doping becomes increasingly difficult with higher Aluminium content of the AlGaN layers as required for ultra-violet light emission.

Significant built-in polarization charges are known to occur at all hetero-interfaces of nitride-based devices. The reason is the high spontaneous and strain-induced polarization in nitride semiconductor materials, which depends on the material composition. By continuously grading this composition, a fixed density of negative bulk polarization charges can be generated. Such graded AlGaN layers were recently demonstrated to enhance the density of free holes substantially, both for N-face growth (Simon et al. 2010) and Ga-face growth

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(Zhang et al. 2010). Ga-face is the conventional LED growth method. The novel N-face growth method reverses the direction of the built-in polarization field so that polarization-induced hole doping can be advantageously combined with an increasing band gap of the p-AlGaN layer (Simon et al. 2010).

For the first time, this paper compares the effect of Ga-face and N-face graded p-AlGaN layers on the performance of ultra-violet (UV) LEDs. Advanced device simulation software is used as main tool of this investigation (APSYS).

2 Models and parameters

The one-dimensional LED simulation self-consistently solves the semiconductor carrier transport equations, coupled to the photon emission from the strained AlGaN quantum wells. Schrödinger and Poisson equations are solved iteratively in order to account for the quantum well deformation with changing device bias (quantum-confined Stark effect). The transport model includes drift and diffusion of electrons and holes, Fermi statistics, built-in polarization and thermionic emission at hetero-interfaces, as well as non-radiative recombination of carriers. The non-radiative carrier lifetime strongly depends on the growth quality, we here use a uniform value of 1 ns.

The built-in polarization charge density is calculated using the Bernardini model (Bernardini 2007) assuming 50% compensation by charged defects (Piprek and Li 2010). Due to the typical n-type background doping of AlGaN, low Mg doping is applied in the simulation, giving an acceptor density of $N_A = 10^{17}cm^{-3}$ in the graded layer. The Mg acceptor activation energy varies linearly with the AlGaN composition, it is 170 meV for GaN and 470 meV for AlN. The carrier mobility strongly depends on composition and doping. The exact value of the mobility is hard to predict, especially for holes. For simplicity, we here employ a constant mobility of 5 cm^2/Vs for holes and 100 cm^2/Vs for electrons. The unstrained room-temperature $Al_xGa_{1-x}N$ energy band gap is calculated using

$$E_g(x) = xE_{AlN} + (1 - x)E_{GaN} - x(1 - x)E_{bow} \quad (1)$$

with $E_{AlN} = 6.28\,eV$, $E_{GaN} = 3.42\,eV$, and $E_{bow} = 0.7\,eV$. As the bandgap increases with rising Al mole fraction, the AlGaN band offset ratio between conduction band edge (E_c) and valence band edge (E_v) is $\Delta E_c : \Delta E_v = 50 : 50$ (Piprek 2010).

Photon extraction from the LED chip and LED self-heating are neglected in this study since we analyze internal mechanisms in pulsed operation. Further details on models and parameters can be found elsewhere (Piprek and Li 2005).

3 Simulation results

The UV LED design example used in this study is based on a recently published device structure with three 1.5-nm-thick undoped $Al_{0.62}Ga_{0.38}N$ quantum wells (QWs) separated by 6-nm-thick undoped $Al_{0.77}Ga_{0.23}N$ barriers and emitting at 250 nm wavelength (Hirayama et al. 2010). The multi-quantum well (MQW) active region is grown on a 2-μm-thick Si-doped $Al_{0.77}Ga_{0.23}N$ buffer layer. Correspondingly, the lattice constant considered in the calculation is a = 3.13 Å for the entire structure. In this Section, the p-side of the original device is replaced by a 50 nm thick graded p-AlGaN layer with different grading direction for Ga-face growth and N-face growth, respectivley (Fig. 1).

First, the conventional Ga-face growth method is investigated, which requires a decreasing Al content of the graded layer to generate negative bulk polarization charges. Grading

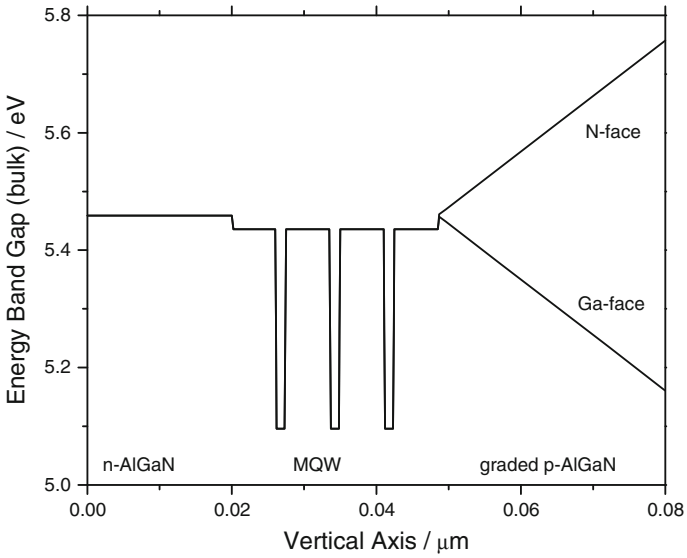

Fig. 1 Vertical profile of the energy band gap for the two LED structures investigated

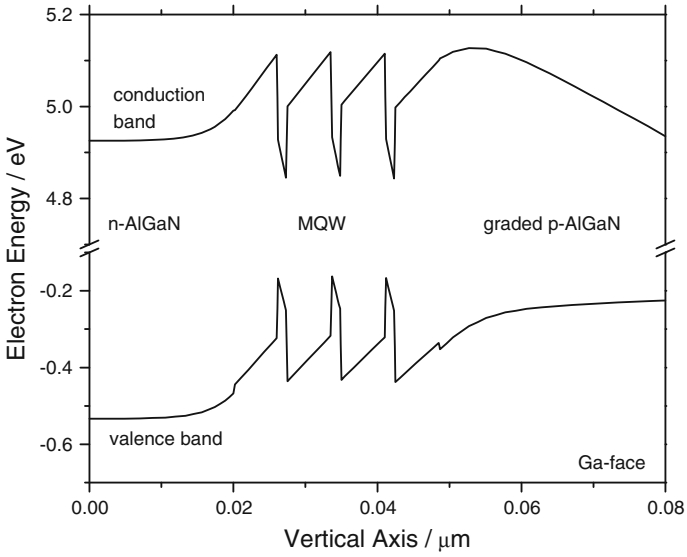

Fig. 2 Vertical energy band diagram for the Ga-face LED ($j = 200\,A/cm^2$)

the Al mole fraction from 0.77 to 0.59 results in a fixed charge density of $1.1 \times 10^{18}\,cm^{-3}$. Figure 1 plots the bulk band gap and Fig. 2 shows the energy band diagram for the Ga-face LED structure at $j = 200\,A/cm^2$ current density. The AlGaN band gap decreases toward the p-contact, causing a potential barrier for hole injection. As typical for Ga-face growth, the n-side QW interfaces exhibit a negative polarization charge while the p-side QW interface is positively charged, leading to a strong deformation of the quantum well.

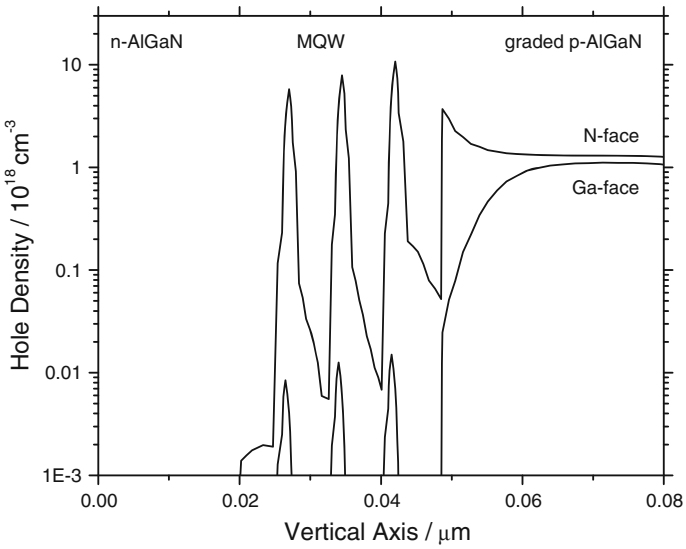

Fig. 3 Vertical profile of the hole density for both LED structures (j = 200 A/cm^2)

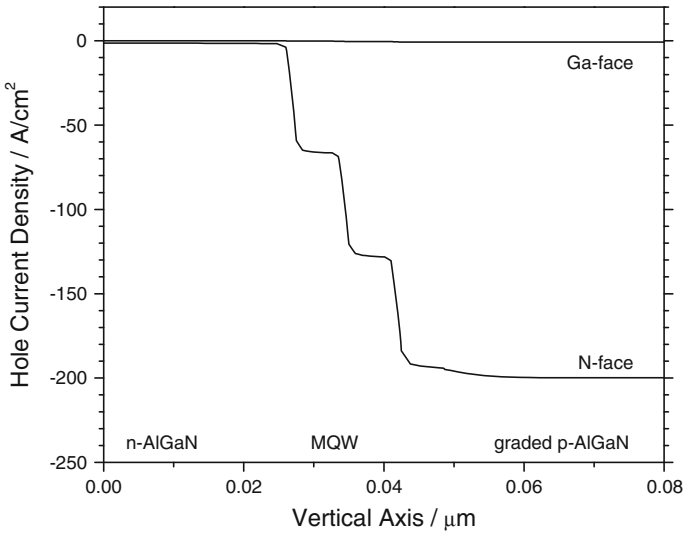

Fig. 4 Vertical profile of the hole current density for both device types. The difference to the total current density of −200 A/cm^2 is equivalent to the electron current density. All those numbers are negative since the holes flow down and electrons up in this simulation

The lower curve in Fig. 3 shows the corresponding hole distribution in the Ga-face device. The negative polarization charge of the graded layer attracts a free hole density of more than 10^{18} cm^{-3} which is about three orders of magnitude above the Mg-induced hole density. However, the hole density in the quantum wells is very small in this case, indicating poor hole injection. Indeed, Fig. 4 shows that the hole current entering the MQW is much smaller than the total current in case of the Ga-face LED, i.e., most holes recombine with leaking

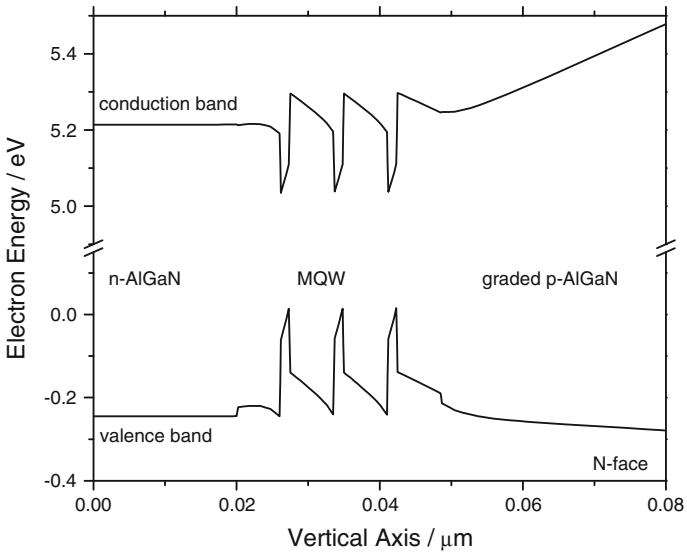

Fig. 5 Vertical energy band diagram for the N-face LED (j = 200 A/cm^2)

electrons on the p-side of the device. In other words, electron leakage is by far the strongest carrier loss mechanism in this case, as the electron current leaking into the p-side of the device is almost as large as the total injection current.

We now move to the N-face case, which can be accomplished in the simulation by simply reversing the sign of the built-in polarization charges. But the grading must also be changed to maintain a negative bulk polarization charge. The Al mole fraction is now increased from 0.77 to 0.95 giving a fixed charge density of 1.3×10^{18} cm^{-3}—slightly higher than in the Ga-face case which is partially due to the different strain. The AlGaN band gap now increases toward the p-contact (Fig. 1). Figure 5 shows the energy band diagram of the N-face structure. The n-side QW interfaces exhibit a positive polarization charge while the p-side QW interface is negatively charged, reversing the QW deformation of the Ga-face LED in Fig. 2. The hole density in the graded layer now peaks near the MQW and then approached the density of fixed charges (upper curve in Fig. 3). The hole density in the quantum wells is much higher than in the Ga-face LED. This more efficient hole injection is confirmed by the lower curve in Fig. 4 which indicates that the electron leakage current into the p-side is negligible.

4 Discussion

The much stronger MQW hole injection in the N-face case is based on two main advantages over the Ga-face LED. First, the p-AlGaN bandgap is lowest at the MQW, allowing for enhanced hole accumulation near the quantum wells (see Figs. 1 and 3). Second, the N-face case does not exhibit an energy barrier in the valence band (Fig. 5) while the Ga-face LED shows such a barrier of about 0.2 eV (Fig. 2).

The calculated internal quantum efficiency (IQE) is listed in Table 1 for various design options. As expected, the N-face LED exhibits the largest efficiency in this list (#1). Still, the IQE value of 0.1 indicates that only one photon is produced per every ten injected electron-hole pairs. The remaining nine electron-hole pairs recombine non-radiatively due to the

Table 1 Internal quantum efficiency (IQE) calculated for various LED design options at $j = 200\ \mathrm{A/cm^2}$ (N_A—acceptor density, x—Al mole fraction in AlGaN, EBL—25 nm thick electron blocking layer with x = 0.95 covered by a 25 nm thick $Al_{0.77}Ga_{0.23}N$ layer)

#	Growth	p-side design (default $N_A = 10^{17}\mathrm{cm}^{-3}$)	IQE
1	N-face	50 nm grading x = 0.77− 0.95	0.1
2	Ga-face	50 nm grading x = 0.77− 0.59	1×10^{-5}
3	Ga-face	50 nm grading x = 0.95− 0.77	0.021
4	Ga-face	EBL	0.023
5	Ga-face	EBL, $N_A = 10^{19}\mathrm{cm}^{-3}$	0.046
6	Ga-face	No grading (x = 0.77)	3×10^{-6}
7	Ga-face	No grading (x = 0.77), $N_A = 10^{19}\mathrm{cm}^{-3}$	3×10^{-3}
8	Ga-face	No grading (x = 0.77), $N_A = 10^{20}\mathrm{cm}^{-3}$	0.07

short non-radiative carrier lifetime assumed in the simulation (1 ns). Increasing this lifetime to 100 ns would result in IQE = 0.9 for the N-face LED.

The initial Ga-face design results in a very low efficiency (#2 in Table 1). However, since Ga-face is the established and preferred growth method, we now explore other Ga-face LED design options to maximize the IQE. Row #3 in Table 1 shows that a higher Al mole fraction in the graded AlGaN layer gives a much enhanced IQE since electrons leaking from the MQW now face a significant energy barrier. The same effect is typically achieved without any grading by inserting an electron blocker layer (EBL) above the MQW (#4). Higher Mg-doping can further enhance the EBL effect but it is hard to achieve in UV-LEDs (#5). For comparison, the last three rows of Table 1 list the IQE for a uniform p-$Al_{0.77}Ga_{0.23}N$ layer with different acceptor densities. The highest acceptor density of $N_A = 10^{20}\mathrm{cm}^{-3}$ is practically out of reach but it would give the highest IQE of all Ga-face LED designs listed. However, N-face growth of a graded AlGaN layer still promises better LED performance than conventional Ga-face growth.

5 Summary

Advanced numerical device simulation is employed to investigate polarization-induced AlGaN hole doping in ultra-violet light emitting diodes and to compare two different growth directions, conventional Ga-face growth and novel N-face growth. While both LED types can produce a high density of free holes in a graded AlGaN layer, N-face growth is found to enable a much higher internal quantum efficiency, even higher than with a conventional electron blocking layer.

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APSYS by Crosslight software. www.crosslight.com

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