AlGaN polarization doping effects on the efficiency of blue LEDs

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The development and application of nitride-based light-emitting diodes (LEDs) is hindered by the low hole conductivity of Mg-doped layers. As an alternative, polarization-induced hole doping of graded p-AlGaN layers was recently demonstrated. Using previously manufactured 440nm LEDs as device examples, this paper evaluates the effect of polarization doping by advanced numerical device simulation, both for Ga-face and N-face growth. Recently published material parameters are employed in the simulation, including new data for the Auger coefficients. The simulations reveal that Auger recombination is the main carrier loss mechanism in these devices, electron leakage seems to exert a much smaller influence on the internal quantum efficiency. The importance of internal physical mechanism is studied in detail, including the Poole-Frenkel field ionization of Mg acceptors, which is commonly held responsible for polarization doping effects. Surprisingly, we find that the field ionization inside the graded p-AlGaN layers is not stronger than in conventional electron blocking layers.

Keywords: gallium nitride, AlGaN, p-doping, compositional grading, polarization charges, light-emitting diode, efficiency, electron leakage, hole injection, Auger recombination, numerical simulation

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. As an alternative, polarization-induced hole doping of graded AlGaN was recently demonstrated, both for N-face growth[1] and Ga-face growth.[2,3] 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 energy band gap of the p-AlGaN layer.

Previously, we have simulated AlGaN polarization doping effects on ultra-violet (UV) LEDs emitting near 240nm.[4] Such UV-LEDs have not been fabricated yet. In this paper, we analyze recently manufactured polarization-doped LEDs emitting near 440nm (Ga-face),[3] and we compare these results to N-face blue LEDs. APSYS device simulation is the main tool of this investigation.[5]

2. MODELS AND PARAMETERS

Our one-dimensional LED simulation self-consistently solves the semiconductor carrier transport equations, coupled to the photon emission from the strained InGaN 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, QCSE). 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 Shockley-Reed-Hall (SRH) recombination and Auger recombination of carriers. The SRH carrier lifetime depends on the growth quality, we here use a uniform value of 50 ns. The influence of Auger recombination within the quantum wells (QWs) of GaN-based LEDs is currently subject to intense debate.[6] We

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here employ recently published values for the bulk InGaN Auger coefficients (C_n=0.7 10^{-31}cm^6/s, C_p=1.4 10^{-31}cm^6/s) which are derived from first-principle computations of indirect Auger processes, mediated by electron-phonon coupling and alloy scattering.[7] These coefficients are much larger than previously calculated values for direct Auger recombination,[8] but they are still about ten times smaller than the Auger coefficient indirectly extracted from measurements on blue LEDs.[9] Direct measurements of the InGaN Auger coefficient have not been published yet.

The built-in polarization charge density is calculated using the Bernardini model [10] and assuming 50% compensation by charged defects.[11] Since the exact Mg doping density was not specified for our reference devices,[3] we assume an acceptor density of N_A=10^{19}cm^{-3} in p-GaN and 3x10^{18}cm^{-3} in the p-AlGaN layer. The acceptor density often lies well below the Mg density and it is usually not exactly known. The Poole-Frenkel model for field-enhanced ionization of Mg acceptors is included in our simulation, since it is considered the key mechanism in the polarization-induced enhancement of the free hole density in graded AlGaN layers.[1-3] The Mg acceptor activation energy varies linearly with the AlGaN composition, from 200meV for GaN to 630meV for AlN.[1] The activation energy of the Si donor is 15meV.[1] 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 hole mobility of 10 cm^2/Vs.

The unstrained room-temperature energy band gap for $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$, respectively, is calculated using

$$E_g(x) = x\,E_{InN} + (1-x)\,E_{GaN} - x\,(1-x)\,E_{b1} \quad (1)$$

$$E_g(x) = x\,E_{AlN} + (1-x)\,E_{GaN} - x\,(1-x)\,E_{b2} \quad (2)$$

with E_{InN} = 0.77eV, E_{GaN} = 3.42eV, E_{AlN} = 6.28eV, E_{b1} = 1.43eV and E_{b2} = 0.7eV. The conduction band offset ratio $\Delta E_c/\Delta E_g$ at hetero-interfaces is also an important parameter in GaN LED simulations. This is true especially for the AlGaN offset as it controls the electron leakage across the AlGaN electron blocking layer (EBL).[12] Offset values are mainly reported for interfaces between binary materials and results vary considerably. We here use $\Delta E_c/\Delta E_g$=0.57 which is close to data measured on ternary alloys.[13,14]

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.[11]

3. CONVENTIONAL LED WITH ELECTRON BLOCKING LAYER

We first simulate the performance of a conventional LED with a 40nm thick $Al_{0.15}Ga_{0.85}N$ electron blocking layer (EBL).[3] The multi-quantum well (MQW) active region is grown on 3-µm-thick Si-doped GaN and consists of eight 3-nm-thick undoped InGaN quantum wells and nine 12-nm-thick undoped GaN barriers and it emits at 440nm wavelength. The exact composition of the QW was not given, but the emission wavelength corresponds to 16% Indium in our QW simulation. The EBL is grown on top of the MQW followed by 110nm p-doped GaN.

Figure 1 shows the energy band diagram near the active region. The quantum wells are strongly deformed due to interface polarization charges. Positive polarization charges are located at the p-side QW interface, pulling the QW electrons towards the p-side. Negative polarization charges are located at the n-side QW interface, pulling the QW holes towards the n-side. This separation of electrons and holes within the quantum wells results in reduced spontaneous emission rates. The relatively strong Mg doping of the EBL (N_A = 3 x 10^{18} cm^{-3}) leads to the compensation of the positive polarization charges at the MQW/EBL interface as well as to significant bending of the conduction band edge inside the EBL. This band bending raises the energy barrier for electrons and it reduces the electron leakage current across the EBL significantly.[12] The calculated electron leakage current is only 0.3% of the total current (j=200 A/cm^2).

Still, the calculated internal quantum efficiency (IQE) characteristic shows some efficiency droop with higher current (solid line in Fig. 2). This efficiency droop is caused by Auger recombination, which can be easily verified by removing Auger processes from the simulation (dotted line in Fig. 2). Removing SRH recombination from the model has a quite different effect (dashed line in Fig. 2) as it increases the peak efficiency and the subsequent efficiency droop. Even more

dramatic IQE effects result from the removal of the Poole-Frenkel field-enhanced ionization of Mg acceptors from the model (dash-dot line in Fig. 2). The electrostatic field inside the EBL peaks at more than 300 kV/cm and a strong effect on the Mg acceptor ionization rate is expected. Figure 3 plots the conduction band edge near the EBL with (solid) and without (dash-dot) field-ionization of Mg acceptors. Without Poole-Frenkel effect, the lower density of ionized acceptors inside the EBL leads to weaker screening of the positive polarization charges at the MQW/EBL interface as well as to less band bending inside the EBL. Both these effects lower the EBL energy barrier by about 100meV and lead to a strong enhancement of the electron leakage current across the EBL (now 70% of the total current), which is reflected in a strong efficiency droop (dash-dot line in Fig. 2). Thus, field ionization of Mg acceptors plays an important role in conventional LEDs, even without polarization doping.

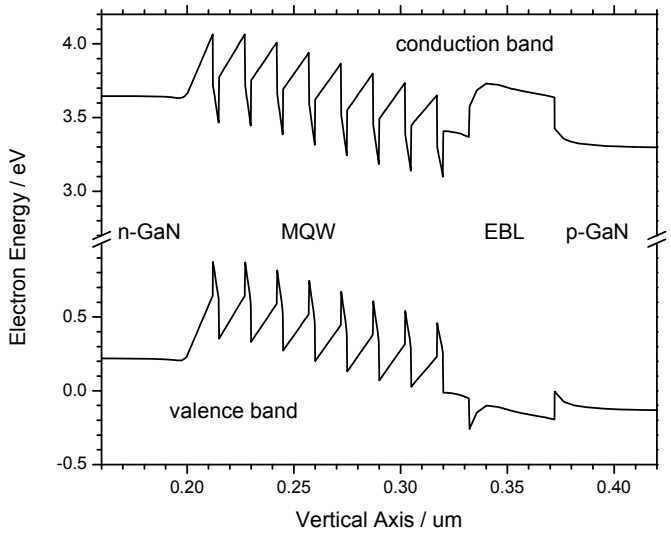

Figure 1 Energy band diagram of the conventional LED at j=200 A/cm^2 current density with multi-quantum well (MQW) active region and AlGaN electron blocking layer (EBL).

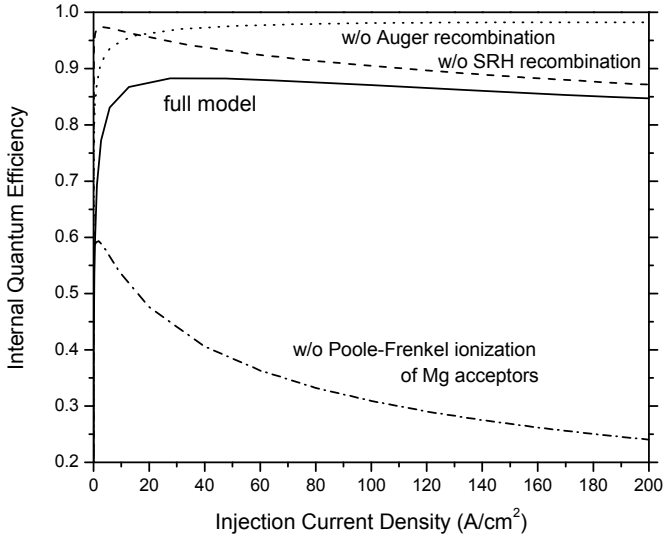

Figure 2 IQE characteristics of the conventional LED with EBL as calculated with different model simplifications.

A quantitative comparison with published IQE measurements on this conventional LED structure is not possible since that publication only shows qualitative efficiency characteristics.[3] However, the measured efficiency droop is similar to the simulation and the measured device bias of 3.45V at 80 A/cm^2 is close to the calculated value of 3.5V. The bias difference may be caused by a slight underestimation of the Mg acceptor density in the model.

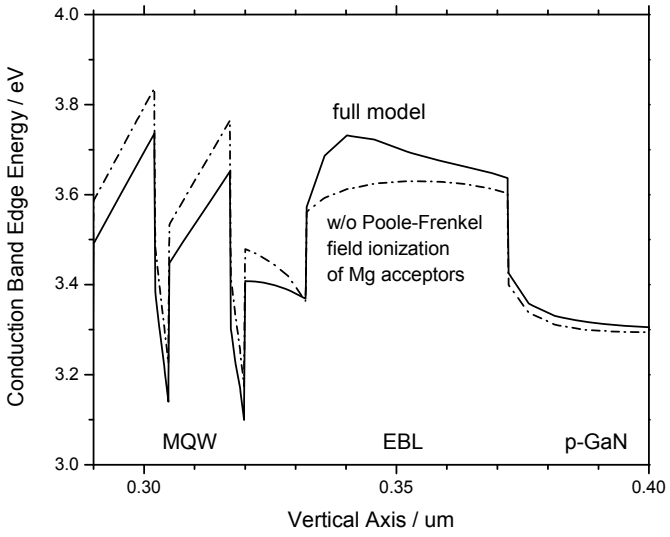

Figure 3 Vertical profile of the conduction band edge as calculated with and without Poole-Frenkel effect at j=200 A/cm^2 current density.

4. CONVENTIONAL LED WITH POLARIZATION-DOPED LAYER

Zhang et al. replaced the EBL with a 40 nm graded p-AlGaN layer of the same Mg doping.[3] We now do the same in the simulation. For proper comparison, we simulate a grading from 15% to 0% Al which has the same conduction band offset as the $Al_{0.15}Ga_{0.85}N$ EBL. Figure 4 shows the energy band diagram of this LED structure. The AlGaN bandgap shrinks towards the p-GaN layer and the band offset to that top layer disappears. This seems to enable better hole injection into the MQW, however, the hole injection rate with the original EBL was already 99.7%, so not much IQE improvement is expected here. Indeed, the IQE characteristic shown in Fig. 5 is almost identical to the IQE curve of the original LED with traditional EBL. In fact, the IQE at j=200 A/cm^2 is slightly lower than before which is caused by a slightly higher electron leakage current of 3%. This leakage is caused by the slightly lower energy barrier in the conduction band of the graded layer (Fig. 4). Further reduction of this barrier by the removal of the Poole-Frenkel effect leads to even stronger efficiency droop (dash-dot line in Fig. 5).

In our model, the AlGaN grading translates into the density N_{pol}= 7.8 x 10^{17} cm^{-3} of negative bulk polarization charges. Other models suggest higher values, e.g., N_{pol}= 18.8 x 10^{17} cm^{-3}.[1] Using this higher value results in the dashed IQE curve in Fig. 5 which is quasi identical to the IQE characteristic of the device with traditional EBL (Fig. 2) since the electron leakage is negligible in both cases. Thus, polarization doping of conventional blue Ga-face LEDs does not lead to significant efficiency improvements. This finding is in good agreement with the experimental investigation of the same LED structures.[3] A direct experimental comparison was made between the $Al_{0.15}Ga_{0.85}N$ EBL and a graded p-AlGaN layer starting with 20% Al, thus giving a slightly better performance. Such performance improvement may have been achieved by simply using an $Al_{0.2}Ga_{0.8}N$ EBL.

The key problem with Ga-face devices is that the graded AlGaN layer must start with the highest Al concentration to generate negative polarization charges, thereby creating a valence band barrier at the MQW/AlGaN interface (Fig. 4). Even in LEDs with poor hole injection, this potential barrier keeps blocking holes from entering the MQW and it makes polarization doping of Ga-face LEDs less advantageous.[4]

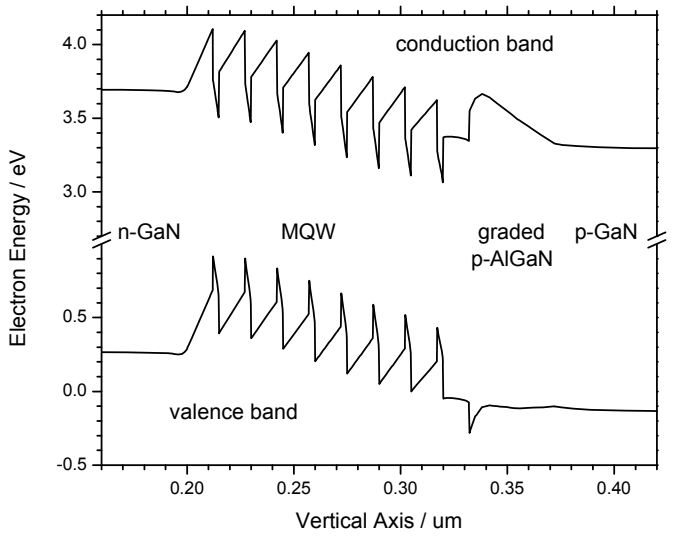

Figure 4 Energy band diagram of the Ga-face LED with graded p-AlGaN layer (j=200 A/cm^2).

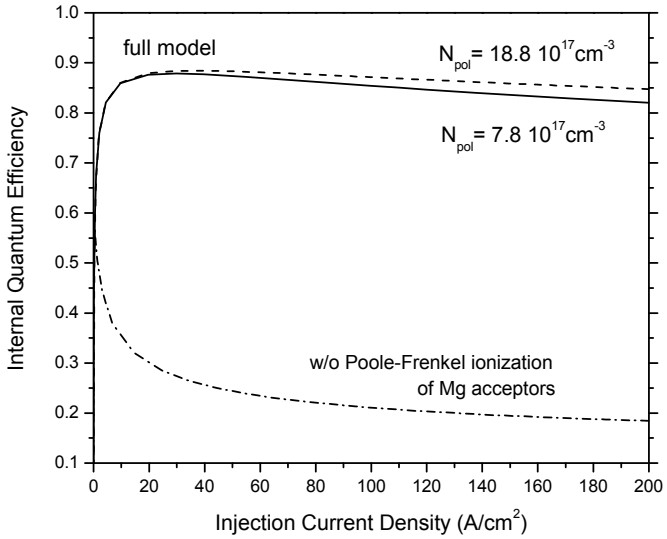

Figure 5 IQE characteristics for the Ga-face LED with polarization doped p-AlGaN layer (N_{pol} – negative polarization charge density in the graded AlGaN layer).

5. N-FACE LED WITH POLARIZATION-DOPED LAYER

The solution to this problem seems to be the growth of N-face structures in which the built-in polarization is reversed.[1] This way, the graded AlGaN layer starts with the lowest Al concentration thereby avoiding the barrier in the valence band. For better clarity, Fig. 6 compares the band gap profiles of all three structures simulated in this study, which only differ above the MQW. The N-face LED features a 40-nm-thick graded p-$Al_xGa_{1-x}N$ layer (x=0...0.15) with is covered by a 110-nm-thick p-$Al_{0.15}Ga_{0.85}N$ contact layer. The acceptor density in both p-doped layers is $N_A = 3 \times 10^{18}$ cm^{-3}. The negative bulk polarization charge density in the graded layer is again $N_{pol} = 7.8 \times 10^{17}$ cm^{-3}.

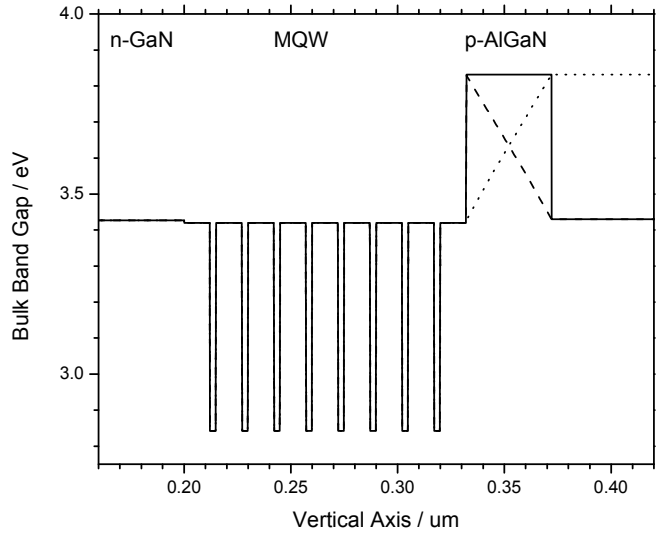

Figure 6 Band gap profile of all three LED structures simulated in this study (solid – Ga-face LED with EBL, dashed – Ga-face LED with graded AlGaN layer, dotted - N-face LED with graded AlGaN layer).

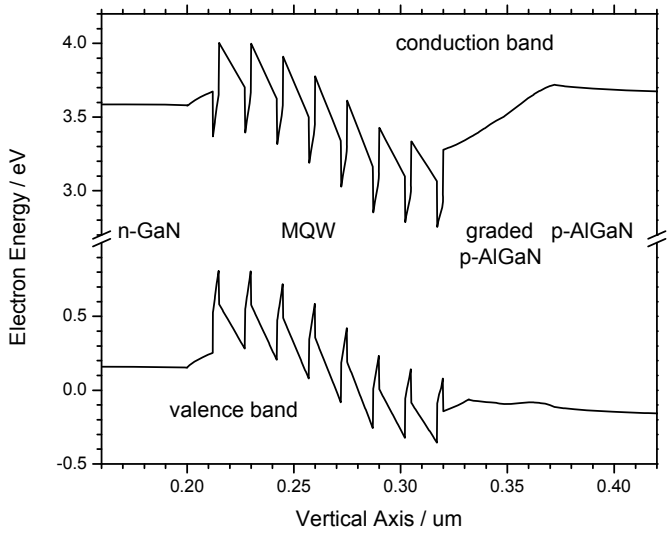

Figure 7 Energy band diagram of the N-face LED with graded p-AlGaN layer (j=200 A/cm^2).

Figure 7 shows the energy band diagram of the N-face LED structure. The valence band barrier in the graded p-AlGaN layer is now eliminated. The conduction band barrier created by this layer now rises gradually and it is not abrupt as in the previous two structures. Significant differences are visible also inside the MQW active region. As the polarization direction is reversed, the negative polarization charges are now located at the p-side QW interface and the positive fixed charges at the n-side QW interface. Obviously, the barriers for electron and hole transport across the MQW have changed significantly, compared to Ga-face growth.

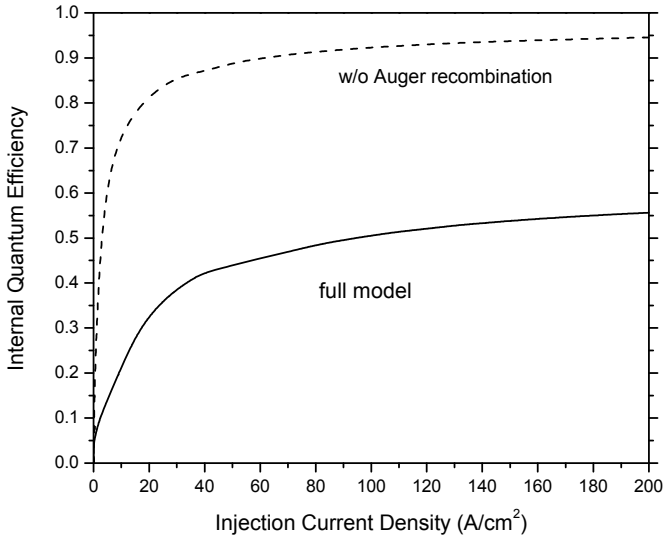

Figure 8 IQE characteristics for the N-face LED with polarization doped p-AlGaN layer.

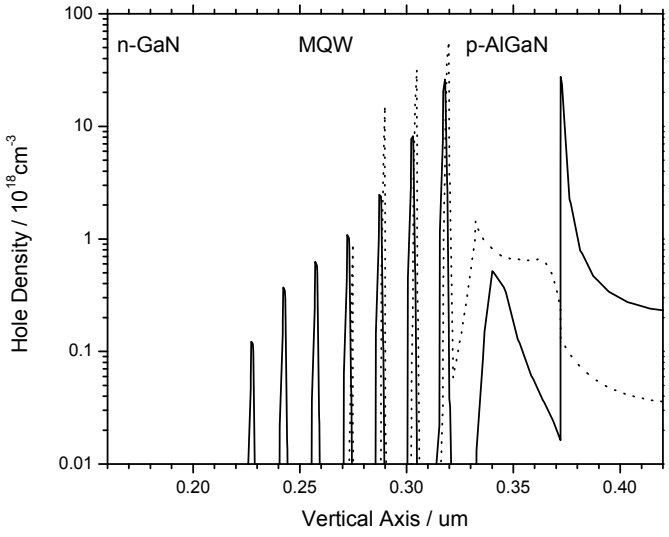

Figure 9 Hole density profile for the N-face LED (dotted line) and the Ga-face LED with EBL (solid line) at j=200 A/cm^2.

The calculated IQE characteristic is plotted in Fig. 8. The efficiency droop has disappeared, however, the IQE at j=200 A/cm^2 is now only 0.56, much smaller than with the Ga-face device examples above. At first thought, electron leakage may be blamed for the low efficiency, but the calculated electron leakage current from the MQW is practically zero and, correspondingly, the hole injection rate into the MQW is 100%. Thus, Auger recombination is the only other carrier loss mechanism that can cause this IQE reduction, since the assumed SRH lifetime is very long (50ns). After removing Auger recombination from the model, the dashed curve in Fig. 8 shows a droop-free IQE characteristic reaching 0.96 at 200 A/cm^2. But how can the Auger effect be so much stronger in N-face devices considering that the same Auger coefficients is used as for the Ga-face devices above ? The answer to this question lies in the carrier distribution among the eight quantum wells. Figure 9 shows the hole density profile both for the N-face LED (solid line) and for the conventional Ga-face LED with EBL (dotted line). Due to the different band-edge profiles, holes are able to move deeper into the MQW of the Ga-face structure than in the N-face structure. Therefore, the N-face structure exhibits an increased hole density in the p-side quantum wells. The situation is similar for electrons (not shown). As the Auger recombination rate scales with the third power of the carrier density, it is about 3 times larger in the p-side QWs of the N-face MQW. In other words, the more uniform MQW carrier concentration in the Ga-face MQW gives a much smaller net Auger recombination than in the N-face case, even for the same total carrier density inside the quantum wells. A similar phenomenon was previously observed in MQW laser diodes.[15]

Figure 9 also shows the intended enhancement of the hole density in the graded p-AlGaN layer which is larger than in the traditional EBL. It is also larger than in the neighboring p-$Al_{0.15}Ga_{0.85}N$ layer despite an identical acceptor density of $N_A = 3 \times 10^{18}$ cm^{-3}. Thus, the negative bulk polarization charges in the graded layer lead to a higher hole density, which is close to the density of bulk polarization charges.

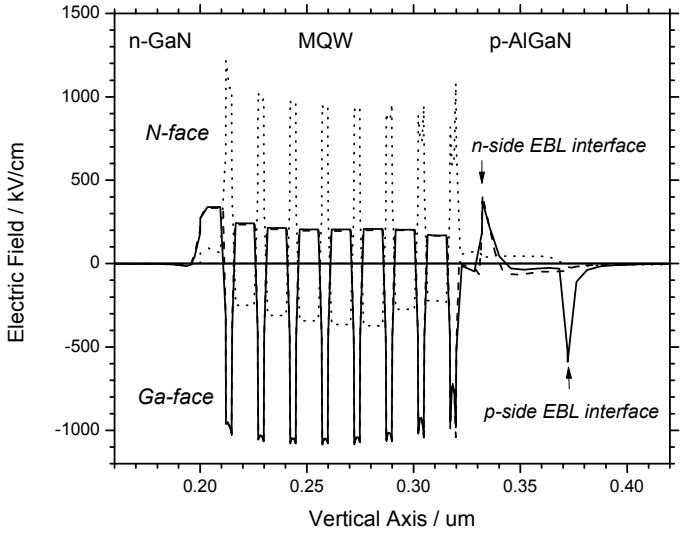

Figure 10 Electric field profile at j=200 A/cm^2 for the Ga-face LED with EBL (solid line), the Ga-face LED with graded layer (dashed line), and the N-face LED (dotted line).

Previous publications claim that the Poole-Frenkel ionization of Mg acceptors by the electric field is responsible for the rise of the hole density in the graded p-AlGaN layer.[1-3] Figure 10 plots the calculated field profile for all three devices simulated. As expected, N-face growth reverses the polarization and the built-in electric field (dotted line) which is most obvious in the MQW region. However, the p-AlGaN graded layer presents a more complicated picture. Both Ga-face devices exhibit an abrupt band gap change near the MQW which is accompanied by a high two-dimensional (2D) positive polarization charge and a peak of the electric field at that interface of more than 300 kV/cm. The 2D

polarization charge at the other EBL interface is negative and causes a field maximum of opposite direction (solid line). The graded p-AlGaN layer in the N-face device is not accompanied by 2D polarization charges and it shows a smaller and more uniform electric field of about 40 kV/cm. The Poole-Frenkel effect only depends on the field magnitude, not on the field direction. With peaks at both interfaces, the average field magnitude is highest in the EBL of the conventional LED and the acceptor ionization rate is also the highest. The N-face graded layer exhibits the lowest acceptor ionization rate, removing the Poole-Frenkel ionization from the model has also no effect on the IQE curves in Fig. 8. Thus, the higher hole density inside the N-face graded layer is not generated by enhanced field ionization but is attracted from outside the graded layer due to the negative bulk polarization charge (cf. Fig. 9).

6. DISCUSSION

The results of nitride LED simulations are very sensitive to changes of key material parameters.[12] We now discuss the influence of such parameters on the results presented above. The IQE is potentially limited by two mechanisms, Auger recombination and electron leakage from the MQW. The latter is synonymous with reduced hole injection into the MQW. In our model, Auger recombination is controlled by the Auger coefficients. Electron leakage strongly depends on the conduction band offsets, the interface polarization, and the acceptor density.

Assuming a weaker Auger recombination would eliminate the efficiency droop (cf. Fig. 2) which is contradicted by measurements. Using larger Auger coefficients would lead to a lower IQE maximum and stronger efficiency droop; however, the key findings of this paper would not change qualitatively since Auger recombination already is the dominating carrier loss mechanism in our simulation.

The electron leakage is very small in all three cases simulated. It would be further suppressed by choosing a larger conduction band offset, weaker built-in polarization, or higher acceptor density. Significant effects can only be expected from changing these parameters in the opposite direction. Our AlGaN conduction band offset of 0.57 is already close to the smallest number published (0.55)[16] and a further reduction would be unfounded. A stronger built-in polarization is predicted by the Bernardini model[10] which would pull down the EBL energy barrier and strongly enhance the leakage current (cf. Fig. 3).[17] However, there is a consensus in the community that practical numbers are about 50% smaller due to compensation by charged defects.[12] Reducing the compensation to 10% gives the IQE curves in Fig. 11 (solid lines) which show a large difference between traditional EBL and graded p-AlGaN layer. Such a large efficiency difference clearly contradicts the measured results for these devices.[3] Lowering the EBL acceptor density would reduce the band bending (cf. Fig. 3) and strongly increase the electron leakage. Our p-AlGaN acceptor density represents only 30% of the nominal Mg density,[18] reducing it to $N_A=10^{18}cm^{-3}$ results in the dashed lines in Fig. 11. Thus, enabling a much stronger electron leakage in the simulation would create a substantial difference between the IQE characteristics of the two Ga-face devices, which is not supported by measurements.[3]

Zhang et al. published simulations of their devices using the same software (APSYS) but different models and parameters.[19] The authors do not discuss the influence of models and parameters on their simulation results and most key parameters are not listed in their paper. Thus, we suspect that they use default APSYS settings, neglecting the large Mg acceptor ionization energy as well as the Poole-Frenkel effect. Their IQE simulation results are different from the results shown above, but the reasons cannot be further evaluated here because of unpublished material parameters.

Our previous simulation of ultra-violet (250nm) AlN-based LEDs resulted in carrier losses dominated by electron leakage.[4] Published data for the AlGaN Auger coefficients at the large QW bandgap of 5eV could not be found and a reasonably small value of $C_n = C_p = 10^{-34}$ cm^6/s was assumed, practically eliminating Auger recombination. The conduction band offset was 0.5.[20] The Mg acceptor density in the graded layer was much lower than above ($N_A = 10^{17}$ cm^{-3}) and Poole-Frenkel field ionization was irrelevant. These parameters result in poor hole injection which can be significantly improved using N-face growth and a graded p-AlGaN layer above the MQW. Ga-face growth of an oppositely graded layer was less promising in that case.

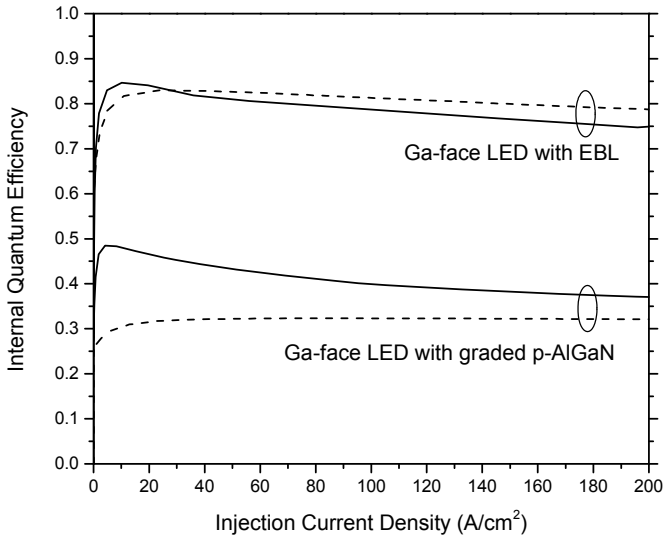

Figure 11 IQE characteristics calculated for the two Ga-face LEDs after reducing the polarization screening from 50% to 10% (solid line) or the acceptor density from $N_A = 3x10^{18}cm^{-3}$ to $1x10^{18}cm^{-3}$ (dashed line).

7. SUMMARY

This theoretical study investigates the effect of polarization doping on internal device physics and quantum efficiency of blue LEDs using practical device examples. As the efficiency in these devices seems to be limited by Auger recombination inside the quantum wells and not by poor hole injection, p-doping enhancement by bulk polarization charges in graded AlGaN layers is unable to further improve the hole injection and the efficiency. The higher hole density in these graded layers is not caused by enhanced field ionization of Mg acceptors, as previously suspected, but rather by electrostatic attraction to the negative bulk polarization charges. Novel N-face growth is found to reduce the LED efficiency compared to conventional Ga-face growth due to poor hole transport inside the MQW.

ACKNOWLEDGEMENT

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