Sensitivity analysis of electron leakage in III-nitride light-emitting diodes

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III-nitride light-emitting diodes (LEDs) suffer from efficiency droop, which is partially attributed to electron leakage into the p-doped layers. Only very few direct measurements of such leakage are published. We here analyze leakage measurements on AlGaN LEDs with an emission wavelength near 260 nm. The electron leakage disappears after insertion of a thin undoped electron blocking layer (EBL). In good agreement with these measurements, we show that the electron blocking effect is extremely sensitive not only to the EBL material composition but also to the conduction band offset and to the net polarization, which are both not exactly known. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4799672]

Light-emitting diodes (LEDs) based on gallium-nitride (GaN) or aluminum-nitride (AlN) are currently of tremendous interest for applications in lighting, displays, sensing, biotechnology, medical instrumentation, and other areas. But the development of III-nitride LEDs is challenged by a strongly declining efficiency with higher injection current, which is observed across the emission spectrum of InGaN/GaN LEDs[1] as well as with ultraviolet (UV) AlGaN/AlN LEDs.[2] The origin of this efficiency droop is still under dispute.[3] The commonly suspected droop mechanisms are Auger recombination inside the active layers[4] and/or electron leakage from the active region into the p-doped layers.[5] However, direct experimental evidence is hard to find for any of these mechanisms and the interpretation of LED efficiency measurements is typically based on modeling.[3] Numerical device simulation tools are often utilized, especially for the analysis of electron leakage and for the design optimization of the AlGaN electron blocking layer (EBL).[5,6] The results of such LED simulations are sensitive to EBL material properties, in particular to composition, doping, polarization, and band offset.[6,7] Some of these parameters are not exactly known, which creates a significant uncertainty in the assessment of electron leakage and in the explanation of the efficiency droop.

Only a few groups published measurements of light emission from the p-doped side of the LED as direct evidence of electron leakage.[8–10] We here simulate and analyze such measurements on UV LEDs, which directly compare the electron leakage before and after placing an EBL between the active region and the p-doped layers.[8] Based on the good agreement with these measurements, our simulation is able to reveal an extremely strong influence of EBL material properties on the electron leakage. Thereby, we intend to stimulate a more realistic discussion of leakage effects on the efficiency droop and to encourage a more accurate experimental determination of these parameters.

Earlier experimental[9] and theoretical[7] studies already discovered a strong leakage current reduction with increasing EBL p-doping (Mg). However, the exact acceptor profile inside the EBL is practically unknown, because only a small part of the Mg atoms is incorporated as AlGaN acceptors,[11] and because the EBL is typically the first p-doped layer in the growth process. Thus, a realistic calculation of electron leakage across a p-doped EBL is difficult. Fortunately, the above cited leakage measurements employed a thin undoped EBL,[8] so that the EBL doping uncertainty is eliminated from our analysis.

The built-in material polarization is known to have a strong effect on III-nitride devices. Its dependence on the material composition results in interface polarization charges, which can be calculated from atomistic models.[12] However, some experimental investigations indicate weaker polarization than predicted.[13,14] This can be attributed to partial compensation of the built-in polarization by charged defects,[15] which are influenced by the growth process. Since the exact compensation ratio is unknown, the polarization charge density is typically scaled down by a fit factor, which is adjusted to find agreement with experimental results, leading to a wide range of reported polarization compensation factors (0.3 to 1).[5,6,16,17]

Rather accurate models are available for the energy band gap E_g as function of AlGaN composition.[18] However, the electron leakage is mainly controlled by the EBL conduction band offset ΔE_c, which is a less known parameter. AlGaN band offset measurements are reported for different compositions and result in a relatively narrow range of offset ratios $\Delta E_c/\Delta E_g$ between 0.55 and 0.65.[19–22] Thus far, almost all published analyses of leakage effects on the LED efficiency droop employ offset values outside this measured range and do not evaluate the impact of this parameter on the simulation results.[5,6,16]

The LED investigated here comprises a multi-quantum well (MQW) active region composed of five 2.8 nm-thick $Al_{0.49}Ga_{0.51}N$ wells and six 5.9-nm-thick $Al_{0.55}Ga_{0.45}N$ barriers.[8] The MQW is sandwiched between a 1 μm-thick n-doped $Al_{0.6}Ga_{0.4}N$ layer and a 25-nm-thick p-doped $Al_{0.6}Ga_{0.4}N$ layer that is covered by a 25-nm thick p-$Al_{0.3}Ga_{0.7}N$ layer and a 200-nm-thick p-GaN layer. Besides the MQW emission peak at a wavelength of 260 nm, the emission spectrum of this LED exhibits a strong second peak above 300 nm that was eventually linked to an acceptor-related emission process.[23] The introduction of a 1-nm-thin undoped AlN EBL eliminates the second emission peak,[8] which directly verifies the suppression

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of electron leakage. The EBL yields a 5-times higher output power at the maximum current density of 30 A/cm^2.[8] The measurement is restricted to a relatively low current, and no significant efficiency droop is observed. In general, strong defect-related recombination is known to cause a low efficiency without efficiency droop.[24] High defect densities are typical for deep UV LEDs,[25] and we assume a relatively short non-radiative carrier lifetime of 1 ns in the following.[26]

Our analysis utilizes the APSYS simulation software,[27] which is widely used to study III-nitride LEDs.[5,6,26,28] The software self-consistently computes the semiconductor carrier transport equations, coupled to the photon emission from the strained quantum wells. Schrödinger and Poisson equations are solved iteratively in order to account for the quantum well deformation with changing device bias. The transport model considers Fermi statistics, drift and diffusion of electrons and holes, thermionic emission at hetero-interfaces, as well as electron and hole tunneling through the thin EBL. The unstrained room-temperature energy band gap for $Al_xGa_{1-x}N$ is $E_g(x) = x\,E_{AlN} + (1-x)\,E_{GaN} - x\,(1-x)\,E_b$ with $E_{GaN} = 3.43$ eV, $E_{AlN} = 6.14$ eV, and $E_b = 0.6$ eV.[18] The initial band offset ratio is 0.6, in the middle of the measured range, and the initial polarization factor is also 0.6 (see discussion below). The EBL material properties are varied in the following to evaluate their impact on the electron leakage. Further details of our models and material parameters can be found elsewhere.[29,30]

Figure 1 depicts the calculated energy band diagram for the device without EBL at 30 A/cm^2 current density. Due to the built-in polarization, the MQW active region deviates significantly from the ideal rectangular shape. The same figure illustrates the current flow. Electrons leaking from the MQW active region into the p-doped side capture holes before they reach the MQW, i.e., electron leakage and reduced hole injection go hand in hand. Without EBL, the electron leakage is mainly controlled by the acceptor density of the p-$Al_{0.6}Ga_{0.4}N$ cladding layer. The acceptor ionization energy scales linearly from 170 meV (GaN) to 470 meV (AlN), and the field ionization is also included in our model.[30] Since the Mg doping density was not specified,[8]

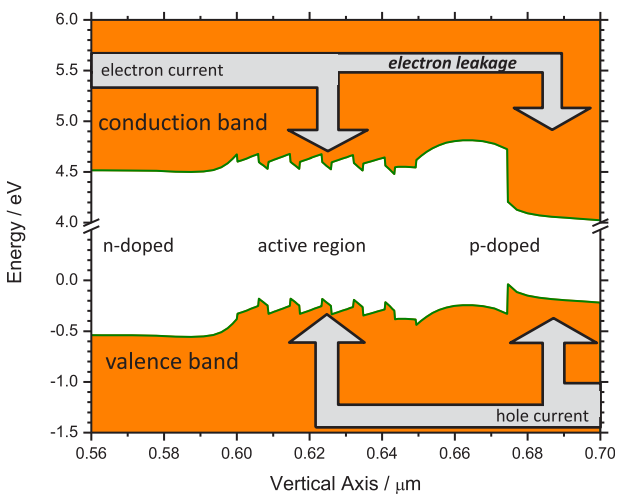

FIG. 1. Energy band diagram of the LED pn-junction at a current density of 30 A/cm^2 with illustration of the electron leakage current from the active region into the p-doped region and the corresponding hole injection.

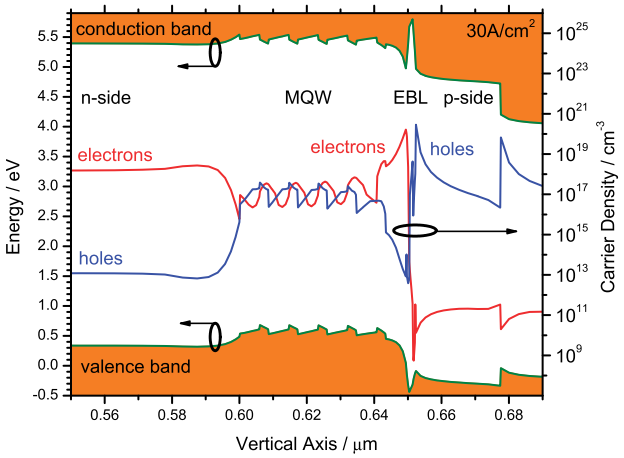

FIG. 2. Vertical energy band diagram and carrier density profiles for the LED with EBL.

we here use it as a fit parameter to match the measured output power enhancement after EBL inclusion. The resulting acceptor density is 1.4×10^{18} cm^{-3}. This relatively low number is reasonable considering the low acceptor formation rate with Mg doping of AlGaN.[11] The fitted acceptor density increases with increasing non-radiative lifetime, however, both parameters have negligible influence on the following analysis of EBL effects.

Figure 2 plots the energy band diagram for the device with EBL as well as the calculated carrier density profiles. On the left-hand-side of the EBL, positive polarization charges attract a high density of electrons, while negative polarization charges on the right-hand-side of the EBL cause a strong hole accumulation. The EBL interfaces are compositionally graded with a grading layer thickness of 1 nm. Without such grading, electron and hole wave functions overlap across the thin EBL and cause another emission peak in the simulation, which is not observed experimentally.[8,23] The EBL grading generates bulk polarization charges with a density of 3.1×10^{20} cm^{-3} on the n-side and 2.8×10^{20} cm^{-3} on the p-side (without fit factor). Figure 3 compares vertical current density profiles. The currents drop steeply within the MQW region due to

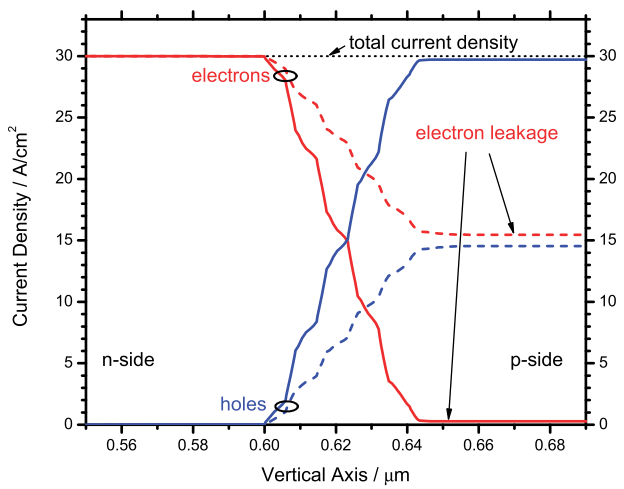

FIG. 3. Current density profiles for electrons and holes calculated with (solid lines) and without EBL (dashed lines).

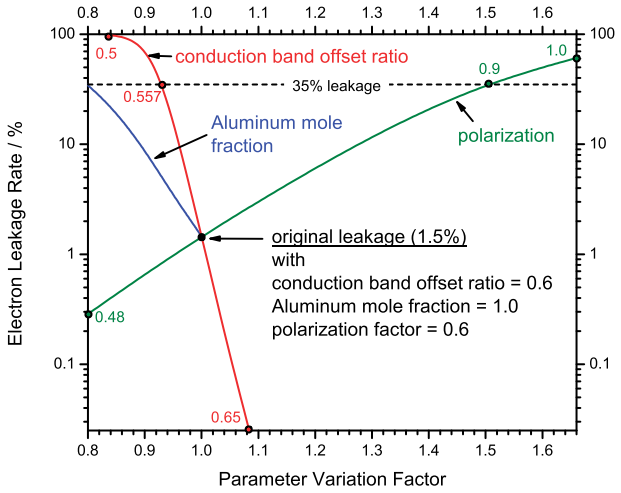

FIG. 4. Effect of parameter variations on the electron leakage rate at a current density of 200 A/cm^2.

radiative and non-radiative recombination of electrons and holes (note that the total current density remains constant). But without EBL (dashed lines), 52% of the injected electrons leak into the p-side. Such leakage disappears almost completely after the EBL is introduced (solid lines). The hole injection rises correspondingly from 48% to 99%, leading to an enhanced light emission from the MQW. Based on the initial offset ratio of 0.6, the polarization factor was lowered to 0.6 in the simulation to achieve the measured suppression of the leakage current.

We now analyze the sensitivity of the electron blocking effect by varying EBL properties in our model. The results are summarized in Fig. 4 for a typical LED current density of 200 A/cm^2. The leakage rate of 1.5% calculated with the initial parameter set is slightly higher than the leakage rate of 1% extracted from the measurement at 30 A/cm^2 (cf. Fig. 3).

Electron leakage turns out to be most sensitive to the conduction band offset ratio. A smaller EBL offset parameter lowers the energy barrier for electron leakage while increasing the energy barrier for hole injection. An offset reduction from 0.6 to 0.5 changes the electron leakage rate from 1% to 98% in Fig. 4. Thus, the strong electron leakage simulated in some publications is mainly due to the low offset ratio of 0.5 used there.[5,16] Other simulations employ a large offset ratio of 0.7 and do not discover any leakage.[31] Note that the absence of electron leakage results in a reduced sensitivity of the LED efficiency to EBL properties. In other words, the insensitivity of the LED efficiency to EBL properties is a strong indication for negligible electron leakage.

More polarization charges lead to enhanced leakage (Fig. 4) because the electron density and the band bending at the EBL are increased (cf. Fig. 2). Full polarization would give a leakage rate near 60%. Assuming full polarization in our initial analysis, a simulation of the reported leakage suppression would require a high offset ratio of 0.72, which is clearly outside the measured range (0.55 to 0.65). At the other and extreme end of the polarization range (no polarization), a low offset ratio of 0.56 is needed for the target leakage rate of 1.5%. While this offset ratio is still within the measured range, the complete compensation of the built-in polarization is an unrealistic assumption for this device. Thus, since the offset ratio is better known than the polarization compensation factor, our approach of picking a mid-range offset ratio of 0.6 and then fitting the polarization factor seems reasonable.

For comparison, we also simulate the influence of the usually well controlled Al mole fraction of the EBL, which affects both the band gap and the polarization charge. Reducing the Al fraction in the EBL to 0.8 results in 35% electron leakage (Fig. 4) since band gap and energy barrier height are reduced. The same leakage rate is calculated with an AlN offset ratio of 0.557 or with an AlN polarization factor of 0.9 (dashed line in Fig. 4). The influence of the Al mole fraction is less dramatic than that of the offset ratio for two reasons: (1) the EBL band gap reduction also improves hole injection; (2) the EBL polarization charges are also reduced, leading to a lower free carrier density at the EBL and less band bending. In other words, the reduction of the offset ratio has such a strong effect in Fig. 4 since it improves electron leakage and simultaneously reduces hole injection. Note that the same leakage rate of 35% is produced by the offset reduction to 0.557 despite a much larger absolute energy barrier ΔE_c for electrons (762 meV) compared to the case with $Al_{0.8}Ga_{0.2}N$ EBL (438 meV). This is not only caused by the 2.5-times higher electron density at the AlN EBL, compared to the $Al_{0.8}Ga_{0.2}N$ EBL, but also by the difference in the EBL valence band barrier ΔE_v (544 meV and 236 meV, respectively). Considering the different Al mole fraction on both sides of the EBL, 0.55 on the n-side and 0.6 on the p-side, the EBL barrier ratio $\Delta E_c/\Delta E_v$ of 1.4 with AlN EBL is smaller than the value of 1.85 obtained with the $Al_{0.8}Ga_{0.2}N$ EBL. Thus, the large AlN electron barrier of 762 meV is counteracted by the higher electron density as well as by the relatively high hole barrier of 544 meV, resulting in the same leakage rate as with $Al_{0.8}Ga_{0.2}N$ EBL.

In summary, we analyze one of the few available direct measurements of the EBL effect on the electron leakage in III-nitride LEDs and find that this effect is very sensitive to EBL material properties, in particular to the band offset ratio, the net polarization charge density, and the composition. Thus, a reliable assessment of electron leakage is difficult without direct measurements, as long as some of these EBL parameters are not exactly known.

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