Establishment of the relationship between the electron energy and the electron injection for AlGaN based ultraviolet light-emitting diodes

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Abstract: This work establishes the relationship between the electron energy and the electron concentration within the multiple quantum wells (MQWs) for AlGaN based deep ultraviolet light-emitting diodes (DUV LEDs). The electron energy of different values can be obtained by modulating the Si doping concentration in the n-AlGaN layer and/or engineering the polarization induced interface charges. The modulated Si doping concentration in the n-AlGaN layer will cause the interface depletion region within which the electric field can be generated and then tunes the electron energy. The polarization induced charges and the polarization induced electric field can be obtained by stepwisely reducing the AlN composition for the n-AlGaN layer along the [0001] orientation. We find that the electron concentration in the MQWs can be increased once the electron energy is reduced to a proper level, which correspondingly improves the external quantum efficiency (EQE) for DUV LEDs. According to our investigations, it is more advisable to adopt the n-AlGaN layer with the stepwise AlN composition, which can make both the EQE and the wall plug efficiency high.

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1. Introduction

Featured with small size, low voltage consumption, easy compatibility with electronic systems (e.g., water purifying system, medical devices), AlGaN based deep ultraviolet light-emitting diodes (DUV LEDs) are deemed as the excellent candidate to replace the conventional mercury based UV light sources, and thus they have attracted extensive research interest [1, 2]. Recently, a 85% internal quantum efficiency (IQE) that is measured by using the low-temperature photoluminescence method has been achieved recently [3]. However, this number merely reflects the improved crystal quality by engineering the defects. Once the DUV LED wafer is fabricated into LED chips for which no surface and encapsulation systems (e.g., water purifying system, medical devices), AlGaN based deep ultraviolet light-emitting diodes (DUV LEDs) are deemed as the excellent candidate to replace the conventional mercury based UV light sources, and thus they have attracted extensive research interest [1, 2]. Recently, a 85% internal quantum efficiency (IQE) that is measured by using the low-temperature photoluminescence method has been achieved recently [3]. However, this number merely reflects the improved crystal quality by engineering the defects. Once the DUV LED wafer is fabricated into LED chips for which no surface and encapsulation
composition for the AlGaN based last quantum barrier for DUV LEDs [11]. Besides increasing the hole concentration level in the MQW region, efforts shall be made to enable the better electron capture efficiency for the MQWs. For achieving that goal, AlGaN/AlGaN MQWs with diminishing barrier thickness from the p-side layer to the n-side layer is suggested [12]; AlGaN quantum barriers with the graded AlN composition also shows the advances in increasing the electron injection efficiency for DUV LEDs [13]. Because of the strong polarization effect occurring at the interface of the last quantum barrier and the p-EBL for the [0001] oriented DUV LEDs, the effective conduction band barrier height for the p-EBL decreases, which can nevertheless become increased and better confine electrons by inserting a properly thin AlN layer [14]. Another proposal to increase the electron concentration across the MQW region is to reduce the thermal energy for electrons, which has shown the effectiveness in improving the electron injection capability for GaN-based blue LEDs [15–18]. Interestingly, the report in [15] demonstrates the origin for the enhanced electron injection for GaN-based blue LEDs by using the AlGaN n-EBL, such that the polarization induced electric field within the [0001] oriented AlGaN n-EBL can reduce the drift velocity and the corresponding kinetic energy for electrons, enabling the improved electron capture rate by the active region. However, DUV LEDs are based on Al-rich AlGaN layers, and considering the difficulty for growing the Al-rich AlGaN n-EBL layer, we are seeking for the alternative solution. In the meanwhile, it is also essential to establish the relationship between the electron energy and the electron injection capability into the MQW region for DUV LEDs.

2. Device architectures and parameters

In order to address the above point, this work proposes to modulate the electron kinetic energy by conducting the doping strategy and/or by utilizing the polarization induced interface charges. The schematic device architecture for the studied [0001] oriented DUV LEDs is shown in Fig. 1(a). All investigated DUV LEDs (i.e., Device 1, Device 2, Device 3, Device 4, Device 5, Device 6 and Device 7) possess the same architecture except the Si doping concentration and/or the AlN composition in the n-AlGaN electron injection layer, since by doing so, the electron energy can be manipulated. In order to better reveal the device performances, we simulate the DUV LEDs with full structures. We use sapphire as the substrate on which the AlN layer is then included. Next, 20-period AlN/Al0.50Ga0.50N superlattices on the AlN layer are adopted. We have the 3 μm thick n-AlGaN layer as the electron injection layer with different electron concentration (n) profiles for the studied devices. The detailed structural information for the n-AlGaN layers are illustrated in Table 1. The DUV photons with the wavelength of ~280 nm are generated by the 5 periods of Al0.45Ga0.55N/Al0.55Ga0.45N MQWs for which the quantum well and the quantum barrier thicknesses are 3 nm and 12 nm, respectively. A 10 nm thick p-Al0.60Ga0.40N EBL is employed to better confine electrons within the MQW region. Lastly, a 50 nm p-Al0.40Ga0.60N/50 nm p-GaN is utilized serving as the hole supplier layer.
Table 1. Structure information of the thickness, the electron concentration and the alloy composition in the n-AlGaN layers for Devices 1 to 7. We stepwisely decrease the AlN composition along the [0001] orientation for Devices 2, 3, 4, 5 and 6.

| Device number (Di) | structure information for the respective n-AlGaN layer |
|--------------------|--------------------------------------------------------|
| Device 1           | n-Al0.18Ga0.82N(3.0µm, n=3×10^{19}cm^{-3})             |
| Device 2           | Al0.59Ga0.41N/Al0.59Ga0.41N junctions(x>y)              |
|                    | n-Al0.69Ga0.31N(2.6µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.75Ga0.25N(0.1µm, n=3×10^{19}cm^{-3})              |
| Device 3           | Al0.59Ga0.41N/Al0.59Ga0.41N junctions(x>y)              |
|                    | n-Al0.69Ga0.31N(2.6µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.75Ga0.25N(0.1µm, n=3×10^{19}cm^{-3})              |
| Device 4           | Al0.59Ga0.41N/Al0.59Ga0.41N junctions(x>y)              |
|                    | n-Al0.69Ga0.31N(2.7µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.75Ga0.25N(0.1µm, n=3×10^{19}cm^{-3})              |
| Device 5           | Al0.59Ga0.41N/Al0.59Ga0.41N junctions(x>y)              |
|                    | n-Al0.69Ga0.31N(2.8µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.75Ga0.25N(0.1µm, n=3×10^{19}cm^{-3})              |
| Device 6           | Al0.59Ga0.41N/Al0.59Ga0.41N junctions(x>y)              |
|                    | n-Al0.69Ga0.31N(2.9µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.75Ga0.25N(0.1µm, n=3×10^{19}cm^{-3})              |
| Device 7           | n-Al0.18Ga0.82N(2.5µm, n=3×10^{19}cm^{-3})              |
|                    | n-Al0.18Ga0.82N(0.5µm, n=3×10^{19}cm^{-3})              |

As is shown in Table 1, we decrease the electron concentration and/or stepwisely reduce the AlN composition along the [0001] orientation for the n-AlGaN electron injection layer, e.g., Al_{x}Ga_{y}N/Al_{x}Ga_{y}N architectures with x>y. On one hand, the different doping concentration within the n-AlGaN layer can cause an interface depletion region, and the electric field in the depletion region is along the [0001] orientation [see Fig. 1(b1), in which the electron concentration for the L2 region is lower than that for the L1 region], which can reduce the kinetic energy for electrons. On the other, the Al_{x}Ga_{1-x}N/Al_{x}Ga_{1-y}N interface possesses the negative polarization induced interface charges that can simultaneously produce the polarization induced electric field. More importantly, the polarization induced electric field on the Al_{x}Ga_{1-x}N side is along the [0001] orientation [e.g., the L2/L3 interface in Fig. 1(b2)] that helps to reduce the kinetic energy for the incoming free electrons. It is shall be noted that the electric field on the Al_{x}Ga_{1-x}N side is opposite to the [0001] orientation [e.g., the L2/L3 interface in Fig. 1(b3)], and the electrons will obtain more energy when traveling through it. Fortunately, the electric field intensity in Fig. 1(b3) is smaller than that in Fig. 1(b2) since the high AlN composition in the Al_{x}Ga_{1-x}N layer causes a smaller dielectric constant, and this enables the even stronger electric field intensity therein [19, 20].
For better calibrating our calculation models, we fabricate Device 1 into chips. Inductively coupled plasma (ICP) etching is used to obtain the $650 \times 320 \mu m^2$ mesa. We adopt Ti/Al metal stack on the n-Al$_{0.58}$Ga$_{0.42}$N layer serving as the n-contact, and the Ti/Al is annealed in N$_2$ for 1 min at the temperature of 900 °C. Ni/Au is employed as the current spreading layer, which is then annealed in O$_2$ for 5 min at the temperature of 550 °C. Lastly, Ti/Al/Ni/Au metals are simultaneously deposited on the Ti/Al alloy and the Ni/Au current spreading layer serving as the n-electrode and the reflective p-electrode, respectively. Flip-chip devices for Device 1 and we collect the DUV photons from the sapphire side by an integrating sphere.

We then conduct numerical calculations by using APSYS [6, 8, 15, 19, 20], which can well solve Poisson equations and Schrödinger equations self-consistently. Import physical parameters include Auger recombination coefficient, Shockley-Read-Hall (SRH) recombination lifetime, the energy band offset ratio for AlGaN/AlGaN heterojunctions and the polarization level for [0001] oriented DUV LEDs, which are set to $1 \times 10^{-30}$ cm$^6$s$^{-1}$, 10 ns, 50:50 and 40%, respectively [8, 10]. The carrier transport is modeled by the drift-diffusion process, and we also consider the thermal-assisted intraband tunneling for the energy barriers in the non-active region (e.g., p-EBL). The light extraction efficiency (LEE) is calculated by utilizing the finite different time domain (FDTD) method, which can take the effect of the refractive index and the absorption coefficient for AlGaN based layers into account [21]. The calculated LEE for all the DUV LEE is ~9%, which number agrees well with the report in [21]. Furthermore, Fig. 2(a) shows the experimentally measured EQE and optical power...
density in terms of the injection current density for Device 1. The experimentally measured values are well reproduced numerically. In addition, the agreement between the measured and the calculated current-voltage characteristics in Fig. 2(b) further confirms the effectiveness of the set physical parameters for our devices.

![Graphs](image)

Fig. 2. (a) Experimentally measured and numerically calculated optical power density and EQE as the function of the injection current density for Device 1 (the LEE is set to 9%), (b) experimentally measured and numerically calculated current density in terms of the applied voltage for Device 1.

3. Results and discussions

Figure 3 selectively presents the energy bands and the electric field profiles within the n-AlGaN layers for Devices 1, 2, 3, and 7 at the current density level of 160 A/cm$^2$, respectively. This current density level is purposely chosen to explore the impact of the electron kinetic energy on the electron injection capability when the device is biased at a very high current density level. Figure 3(a) shows the flat energy band when the electron concentration and the AlN composition are constants in the n-AlGaN layer for Device 1. Besides the energy band, we also illustrate the electric field profile within the n-AlGaN layer. For an even better resolution, we enlarge the energy band and the electric field profiles in the n-AlGaN layer for Device 1 which are presented in Fig. 3(b). The n-AlGaN electron injection layer and the AlGaN quantum barriers (QBs) for Device 1 have the AlN composition of 58% and 55%, respectively. As a result, the negative polarization induced interface charges at the n-AlGaN/QB bend the energy band upwards (see the energy band profile in the vicinity of the 0.8 μm), as has also been explained previously in Fig. 1(b2). In the meantime, the polarization induced electric field is simultaneously generated, which is along the [0001] orientation as show both in Figs. 3(a) and 3(b). Figure 3(c) shows the energy band and the electric field profiles in the n-AlGaN layer for Device 2 that has the stepwisely reduced AlN composition for the n-AlGaN layer. According to Fig. 1, we can get that the Al$_x$Ga$_{1-x}$N/Al$_y$Ga$_{1-y}$N (x>y) interface possesses the negative polarization induced interface charges which produce the polarization induced electric field with the direction pointing along the [0001] orientation [see Fig. 1(b2) and Fig. 3(c)]. Figure 3(d) presents the energy band and the electric field profiles for Device 3, for which the n-AlGaN layer has both the modulated electron concentration and
the AlN composition as illustrated in Table 1. Clearly we can see from Fig. 3(d) that the modulated electron concentration generates the built-in electric field at the position of 0.3 μm. The observation agrees well with our predictions in Fig. 1(b1). Meanwhile, the polarization induced electric field can also be obtained in the range of 0.3 μm to 0.8 μm according to Fig. 3(d). Interestingly, we observe that the electric field profile in the range of 0.3 μm and 0.8 μm for Fig. 3(d) is different than that in Fig. 3(e), such that the polarization induced electric field that opposes to the [0001] orientation is simultaneously produced on the side with the lower AlN composition for the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{y}\text{Ga}_{1-y}\text{N}$ interface. The finding here is also consistent with the analysis in Fig. 1(b3). However, the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer for the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{y}\text{Ga}_{1-y}\text{N}$ junction has a smaller dielectric constant that helps to increase the electric field intensity therein [19, 20]. When compared with the electric field profile in Fig. 3(d), the reduced electric field intensity on the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ side and the visual absence of the electric field on the $\text{Al}_y\text{Ga}_{1-y}\text{N}$ side in Fig. 3(c) are well due to the screening effect by the higher electron concentration in the n-AlGaN electron injection layer for Device 2. Note, the electric field profiles in the n-AlGaN electron injection layers for Devices 4, 5 and 4 are very similar to that for Device 3, and therefore they are not shown here. The energy band and the electric field profile in the n-AlGaN electron injection layer for Device 7 are demonstrated in Fig. 3(e). Besides the aforementioned polarization induced electric field and the energy band bending effect in the vicinity of the 0.8 μm that are caused by the negative polarization induced charges at the n-AlGaN/QB interface, we also calculate the electric field in the vicinity of ~0.3 μm as shown in Fig. 3(e). Such electric field is generated because of the modulated electron concentration as has been explained previously in Fig. 1(b1).

Fig. 3. Energy band and electric field profiles in the n-AlGaN layers for (a) Device 1 in the range of 0.2 μm and 0.8 μm, (b) Device 1 in the range of 0.74 μm and 0.8 μm, (c) Device 2 in the range of 0.2 μm and 0.8 μm, (d) Device 3 in the range of 0.2 μm and 0.8 μm and (e) Device 7 in the range of 0.2 μm and 0.8 μm. Data are calculated at the current density of 160 A/cm². $E_c$, $E_v$, $E_{Fe}$ and $E_{Fh}$ denote the conduction band, the valence band, the quasi-Fermi levels for electrons and hole, respectively. Energy band structures of the MQW regions for Devices 1, 2, 3, and 7 are shown in Fig. 6 in the supplementary material.
Then, by using \( W = e \int_{0}^{l} E_{\text{field}} \cdot dx \), we can calculate the net work (\( \Delta E \)) made for the electrons during the transportation in the AlGaN layers for Device 1 to 7. Here, \( e \), \( l \) and \( E_{\text{field}} \) represent the electronic unit charge, the electric field profiles within the integration range of \( l \). For comparative study, the \( l \) ranges from 0.2 μm to 0.8 μm as illustrated in Figs. 3(a), 3(c), 3(d) and 3(e). \( dx \) means the integration step that has been properly optimized when setting the mesh lines during numerical computations. In our case, the electrons will lose energy if the integral is a positive value. The integrated values for the electric field profiles in the n-AlGaN layers for Devices 1 to 7 are shown in Fig. 4(a). Clearly we can see that the electrons will lose more energy as the descending device number (i.e., from Device 1 to 7) by following our designs in Table 1. The electric field in the L2/L3 interface [i.e., Fig. (b2)] greatly contributes to the energy loss for electrons. The depletion region width in the L2 layer is thickened once the AlN composition in the L2 layer becomes high, [see Fig. 3(c) for Device 7 that has the Al\(_{0.58}\)Ga\(_{0.42}\)N/Al\(_{0.55}\)Ga\(_{0.45}\)N junction], which in turn increases the integration rage of \( l \), thus causing more energy loss for electrons. Further investigation into Fig. 4(a) reveals that the optical power density is increased by ~8.5% when we compare Device 2 with Device 1. The enhanced optical power density is well attributed to the reduced electron kinetic energy that helps to increase the electron capture rate by the MQWs. However, further decrease for the electron energy seems to less affect the optical power density if we compare Devices 2, 3, 4 and 5. We believe the reduced electron concentration in the n-AlGaN layer compensates the reduced electron kinetic energy, and therefore the electron concentration in the MQWs for Devices 2, 3, 4 and 5 do not significantly vary from each. Interestingly, once the electron lose more energy in the case of Device 6, the optical power density becomes lower, since a too much low electron kinetic energy can make electrons less mobile, and this gives rise the reduced electron concentration level in the MQWs for Device 6. The subsequent increase of the optical power density for Device 7 is attributed to the increased vertical resistivity for the n-AlGaN layer, thus improving the current spreading effect [22], though the electrons lose the most energy.

The electron concentration in the n-AlGaN layer significantly affects the electrical conductivity for DUV LEDs. Therefore Fig. 4(b) presents the forward voltage and the wall-plug-efficiency for the investigated DUV LEDs. It is concluded that by reducing the electron concentration, the forward voltage increases. By comparing Devices 3, 4, 5, 6 and 7, we can find that the forward voltage is strongly influenced by the thickness for the n-AlGaN layer with a lower electron concentration. It is very important to keep the n-AlGaN layer that possesses a lower electron concentration thin so that a reduced forward voltage can be obtained provided that the electric field profiles in the AlGaN/AlGaN junctions can be completely maintained. Figure 4(b) also tells that Device 2 can give the highest wall-plug-efficiency thanks to the enhanced optical power density and the low forward voltage. Therefore, we summarize that the DUV LED performance can be mostly improved by adopting the n-AlGaN electron injection layer with the staircased AlN composition.
Next, to show the impact of the electron kinetic energy on the electron concentration level in the MQWs, we selectively choose Devices 1 and 5 for comparison. Device 5 has 0.2 μm thick n-AlGaN layer with the electron concentration of $3 \times 10^{17}$ cm$^{-3}$ according to Table 1. The electron concentration profiles in the n-AlGaN layer for Devices 1 and 5 are shown in Fig. 5(a). The “dips” in the electron concentration profile for Device 5 is attributed to the electron depletion effect by the polarization induced negative changes at the Al$_x$Ga$_{1-x}$N/Al$_y$Ga$_{1-y}$N interfaces (i.e., n-Al$_{0.56}$Ga$_{0.34}$N/n-Al$_{0.54}$Ga$_{0.36}$N and n-Al$_{0.54}$Ga$_{0.36}$N/n-Al$_{0.52}$Ga$_{0.38}$N interfaces for Device 5). The electron concentration levels in the MQWs for Devices 1 and 5 are presented in Fig. 5(b). It shows the higher electron concentration level for Device 5 than for Device 1 in the last four quantum wells, indicating the better electron capture capability by the quantum wells. We attribute the improved electron capture capability to the less mobile electrons as illustrated in Fig. 4(a). The lower electron concentration in the 0.2 μm thick n-Al$_{0.56}$Ga$_{0.34}$N/n-Al$_{0.54}$Ga$_{0.36}$N/n-Al$_{0.52}$Ga$_{0.38}$N layer suppresses the electron diffusion into the first quantum well, as the result of which Device 5 has a lower electron concentration level in the first quantum well than Device 1. The radiative recombination rate in the MQWs for Device 5 is stronger than that for Device 1 as is shown in Fig. 5(c). The enhanced radiative recombination rate in the last four quantum wells for Device 5 agrees well with Fig. 5(b). Thanks to the reduced AlN composition in the n-AlGaN layer that is adjacent to the MQW region, the reduced polarization induced electric field can be achieved in the first quantum well, which in turn improves the radiative recombination in the first quantum well for Device 5. Furthermore, our calculations also show that the last four quantum wells have the same electric field intensity for Devices 1 and 5 (results not shown here).
4. Conclusions

To summarize, this work has proposed DUV LEDs with modulated AlN composition and/or electron concentration for the n-AlGaN electron injection layer. By stepwisely reducing the AlN composition or decreasing the electron concentration in the n-AlGaN electron injection layer, the electron kinetic energy can be decreased so that the MQW can have more chances of capturing the incoming free electrons. We also find that, by properly reducing the AlN composition and/or decreasing the electron concentration for the n-AlGaN electron injection layer, the optical power density can be enhanced, which is well ascribed to the improved electron concentration level in the MQWs. It is also reported that the forward voltage and the wall plug efficiency is strongly influenced by the electron concentration in the n-AlGaN layer. This work suggests reducing the AlN composition stepwisely for the n-AlGaN electron injection layer to keep both the better optical power density and the decent wall plug efficiency. We strongly believe the proposed DUV LED structure and the reported device physics in this work are very useful for the community to balance the carrier injection and correspondingly improve the device performance for DUV LEDs.
5. Supplementary material

Figure 6 shows energy bands in the MQW regions.

![Energy bands in MQW regions](image)

Fig. 6. Energy bands in the MQW regions for (a) Device 1, (b) Device 2, (c) Device 3 and (d) Device 7. Data are calculated at the current density of 160 A/cm². $E_c$, $E_v$, $E_{fe}$ and $E_{fh}$ denote the conduction band, the valence band, the quasi-Fermi levels for electrons and hole, respectively.

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