Designing AlGaN-based efficient Ultraviolet Light Emitting Diode

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Abstract

AlGaN-based materials have exhibited considerable potential for fabricating ultraviolet (UV) light-emitting diodes (LEDs) owing to their direct, wide, and adjustable energy bandgap. Those deep-ultraviolet (DUV) and far-ultraviolet light-emitting diodes (LEDs), together with laser diodes(LDs), are essential in many fields such as sterilization, virus elimination, ultraviolet communication, and UV curing, as shown in Fig. 1 below [1]. Because of the various applications, The market for semiconductor DUV light sources is expected to expand explosively with higher device efficiency, and hence the development of high-efficiency high-output DUV-LEDs and LDs is an important task. The band-gap energy of AlGaN (aluminum gallium nitride) covers a wide DUV emission range, from 3.4 eV for GaN to 6.2 eV for AlN, which ensures that the emission spectrum of AlGaN-based LEDs covers the ultraviolet range of 200–365 nm [2] Furthermore, this material has other valuable features, including (1) direct transition-type semiconduction in the entire composition range, (2) the possibility of high-efficiency light emission from quantum wells, (3) the possibility of creating both p- and n-type semiconductors, (4) the hardness of the materials and the long life spans of elements, (5) environmental safety (no arsenic, mercury, lead, and other hazardous components), etc. Thus, AlGaN-based semiconductors are the most promising materials for realization of DUV light-emitting devices.

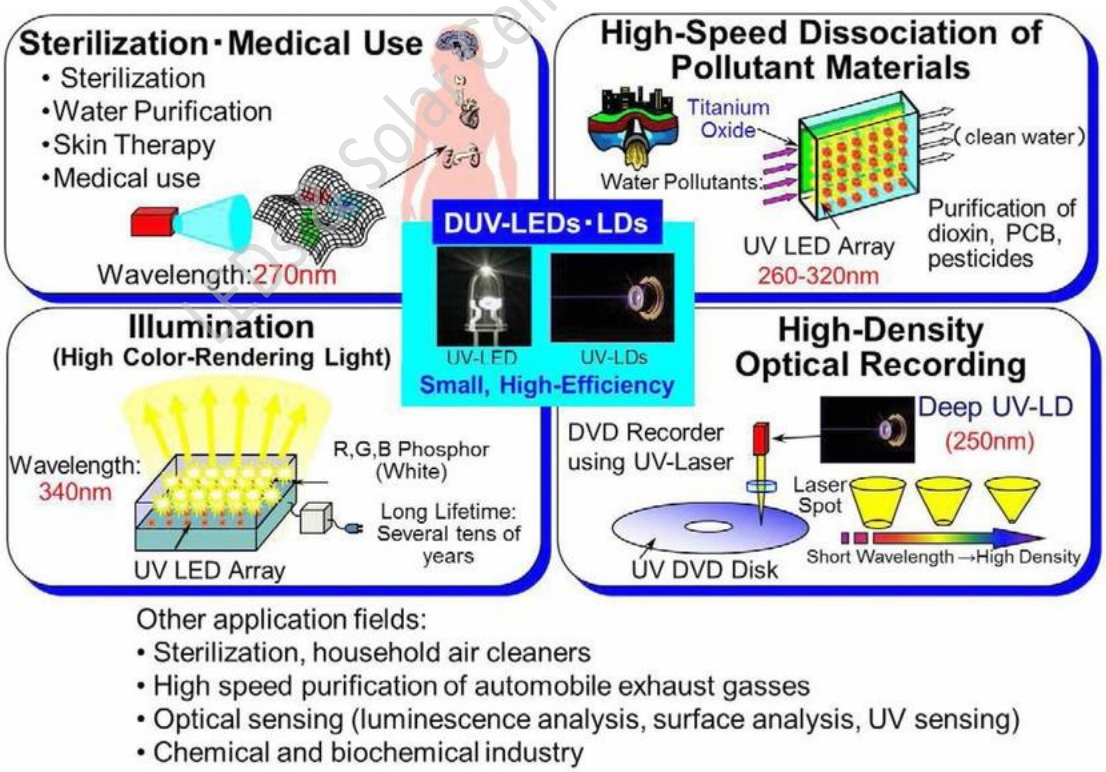

Fig.1 Potential application of DUV LEDs and LDs

Introduction and motivation

In the past decades, to obtain high-performance AlGaN-based LEDs, numerous studies have been dedicated to obtaining high-quality AlGaN-based materials and optimizing the structure of LEDs. Additionally, as shown in Fig. 2 [1], there has been keen competition in the development of DUV-LEDs and LDs with shorter wavelengths and higher efficiency [3]. The development of DUV-LEDs started in about 1997, and the shortest wavelength at the time was about 330 nm. Since 2000, development has been supported by the abundantly funded SUVOP (Semiconductor Ultraviolet Optical Sources) program of DARPA (Defense Advanced Research Projects Agency), and DUV-LEDs with wavelength of 250–280 nm have been implemented [4]. In 2006, the threading dislocation density of AlN crystals was successfully reduced [5], and the DUV internal quantum efficiency (IQE) was improved dramatically. By 2008, short-wavelength LEDs operating at 22–351 nm were realized using high-efficiency light emitting layers [6], and the output reached the practical level of 10 mW and higher. After that, in 2010, multiquantum barriers (MQB) were introduced, and the electron injection efficiency (EIE) was significantly improved. CW outputs above 30 mW can now be obtained. In recent years, there has been keen competition in achieving higher efficiency of DUV-LEDs; in particular, an EQE exceeding 10% was reported [7]. AlGaN-based DUV-LEDs can output several tens to several hundreds of megawatt. The EQE of blue LEDs has exceeded 80%, although the efficiency remains comparatively low. The target is to realize an efficiency of 30% or more, as shown in Fig. 2.

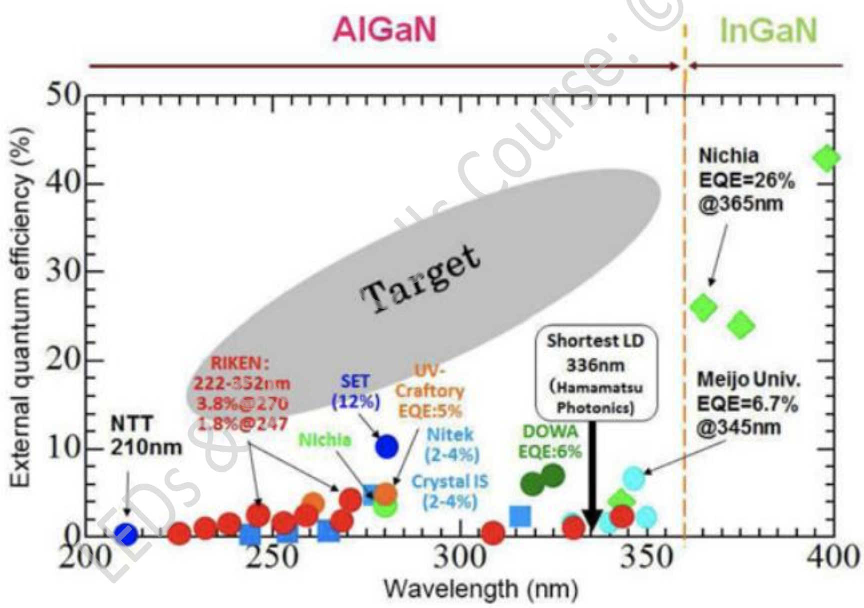

Fig. 2 External quantum efficiency of AlGaN DUV-LEDs

However, AlGaN-based LEDs also have limited applicability because of their low working efficiency, which requires further improvement. This is mainly because of the following reasons: 1) High-quality AlGaN-based materials are difficult to obtain. 2) Highly efficient p-type doping of AlGaN layers is difficult to achieve. 3) The large difference in electron mobility and hole mobility in AlGaN-based materials increases the difficulty of fabricating devices with high injection efficiency for electrons and holes simultaneously. 4) The quantum-confined Stark effect (QCSE) reduces the probability of radiative recombination between electrons and holes. 5) The extremely low light extraction efficiency further decreases the external quantum efficiency (EQE) of AlGaN-based LEDs. 6) It is difficult to obtain AlN with a low threading dislocation density. The IQE of AlGaN light emission is strongly degraded by threading dislocations. In view of these issues, in this report I will mainly talk about the ways to increase the internal quantum efficiency (IQE) and carrier injection efficiency in recent research findings in the fields; and I will use Crosslight simulation to testify those methods' effectiveness.

Technical Background

Just like a basic light emitting diodes, a deep ultraviolet LED consists of a semiconductor p-n junction or QW/MQW sandwiched between a p-n junction. By the mechanism of electroluminescence, light will be emitted when the holes and electrons in the conduction and valence bands recombine radiatively. The QW/MQW can help with the carrier confinement and make the recombination to be more efficient. Generally, depending on the bandgap of the QW material, the emission wavelength of the LED will be determined. However, due to the structure and material characteristics, several other factors can be more important for the recombination efficiency and emission wavelength such as the carrier injection efficiency, the doping level, and the strain effect.

There are several important parameters can be used to evaluate a LED. At first I will introduce the output power. The output power of an LED, denoted by Pout, is the amount of light energy emitted per unit time. The output power is influenced by several factors, including the current supplied to the LED, the semiconductor material, and the device structure. For the UV LED, high power is also demanded in the fields of curing, disinfection, sensing, and sterilization. One equation that can be used to calculate the output power of an LED is

$$P_{out} = \eta_e V I$$

where η_e is the external quantum efficiency, V is the forward voltage, and I is the current supplied to the LED. The external quantum efficiency represents the ratio of the number of photons emitted by the LED to the number of electrons injected into the LED. Another important parameter for the UV LED is the internal resistance. It refers to the resistance that is present within the LED itself, which arises from the physical properties of the semiconductor material used to make the LED. The internal resistance of a UV LED can have a significant impact on its performance. For example, when a voltage is applied across the LED's terminals, some of the electrical energy is converted to heat as it flows through the LED's internal resistance. This heat must be dissipated in order to prevent the LED from overheating and potentially failing. Because of the heat generation, the internal resistance of a UV LED can also affect its efficiency and output power. When a current flows through the LED, some of the electrical energy is converted to UV light, while the rest is dissipated as heat. The efficiency of the LED is determined by the ratio of the UV light output power to the total electrical power input. If the internal resistance is too high, then the electrical power that is available to generate UV light will be reduced, which can result in lower efficiency and output power. Therefore, designing UV LEDs with internal resistances as low as possible is also one of the biggest targets for my project. The internal resistance of a UV LED can be revealed in its IV curve as the one in Fig. 3 shows, which is the reverse of the slope of the IV curve as described by the equation below,

$$R = {}^{dV}/_{dI}$$

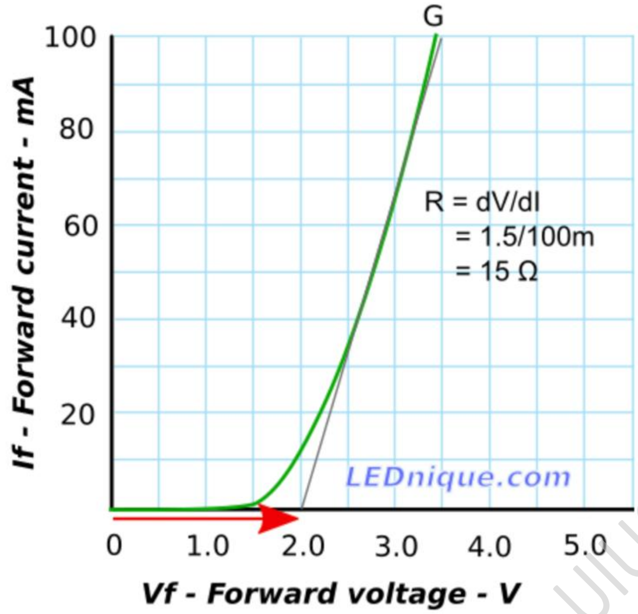

Fig. 3 LED internal resistance example

When excess carriers are injected into an LED, they recombine via various mechanisms. Among these mechanisms, bimolecular radiative recombination is the one we are most interested with since it is the dominate mechanism during the LED electroluminescence process. The parameter that is used to quantify a LED's radiative recombination ability is the internal quantum efficiency (IQE). It is the ratio of the number of photons generated to the number of electrons injected into the LED and is a measure of how drefficiently the LED converts electrical energy into light energy. The internal quantum efficiency, η_i, is influenced by several factors, including the semiconductor material, the device structure, and the operating conditions, which is described by the equation below.

$$\eta_i = \frac{B\Delta n^2}{A\Delta n + B\Delta n^2 + C\Delta n^3}$$

where Δn is the excess carrier concentration and A,B,C are the Shockley-Reed-Hall, radiative and Auger recombination coefficients. The IQE can also be written in terms of the lifetimes of recombination for the radiative and non-radiative processes. τ_{nr} and τ_r would be the non-radiative and radiative lifetimes, we then can then write the internal quantum efficiency η_i as

$$\eta_i = \frac{\tau_r^{-1}}{\tau_r^{-1} + \tau_{nr}^{-1}}$$

Simulation results & Discussion

The simulation of the DUV LED in this project is done through Crosslight. The DUV LED is based on an AlGaN/GaN multiple quantum well structure. It is designed to emit at around 220 nm. The representative structure has a mesa length L_1 of 6 um and L_2 of 1 um while the contacts are half length of the L_1, L_2. The device scale will be calibrated in order to optimize the internal quantum efficiency of the structure. The corresponding Al content in the quantum well is calculated using Vegard's law and is 0.8 for the representative structure. The structure is grown on a AlN substrate because the a-plane lattice constant of AlN is slightly smaller than that of AlGaN-based materials, which is promising for use as a bulk AlN substrate for the growth of AlGaN-based materials. On top of the substrate is a Al_xGaN grading layer that spans the Al composition from 1 to 0.7 in order to reduce the series resistance inside the device and to connect the AlN substrate and the heavily doped $Al_{0.3}GaN$ n-contact (1E19 cm^{-3}). The undoped Al_xGaN grading layer can also be used as a buffer layer to bury all the surface defects and oxides in real growth. The Al composition of the n-contact will be calibrated in order to increase the electron carrier injection and increase the internal quantum efficiency in the device. Another n-type Al_xGaN grading layer is used between $Al_{0.8}GaN$/GaN multiple quantum well and the n-contact to mitigate the strain effect caused by the lattice mismatch. The three quantum well with 5 nm $Al_{0.8}GaN$ active regions are separated by 6 nm undoped GaN barriers. The Al composition in the QW will also be calibrated to optimize the quantum efficiency. On top of QW layers, in symmetry a p-type Al_xGaN grading layer is used to connect with the heavily doped p-type GaN contact layer (1E19 cm^{-3}). The p-contact structure will also be calibrated to increase the hole concentration and internal quantum efficiency of the device. The representative layer structure of the ultraviolet LED is shown in Fig. 4 and the corresponding band diagram is shown in Fig. 5.

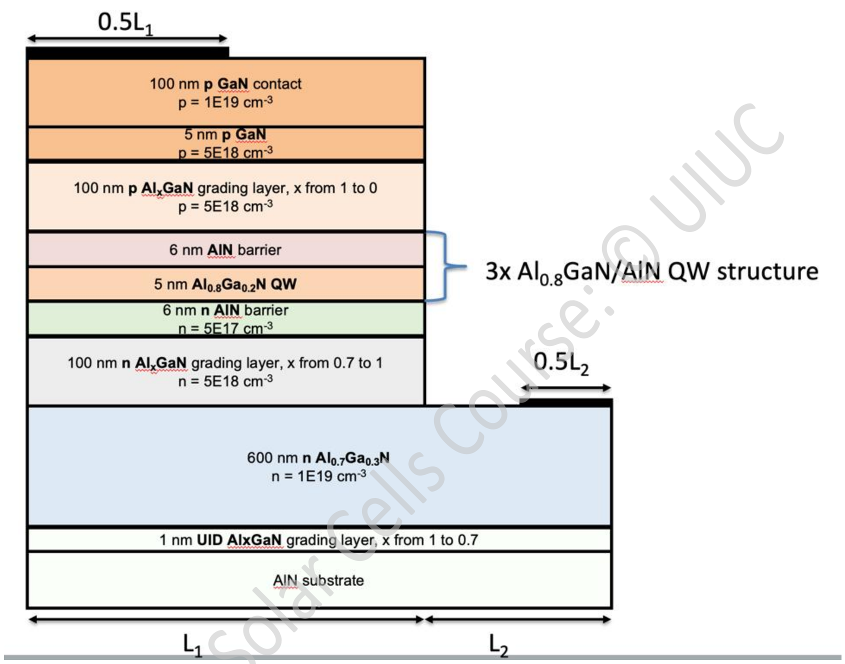

Fig. 4 Ultraviolet LED structure, dimension L_1, L_2 will be scaled. The p contact structure, Al content in the quantum well and the n contact will also be calibrated

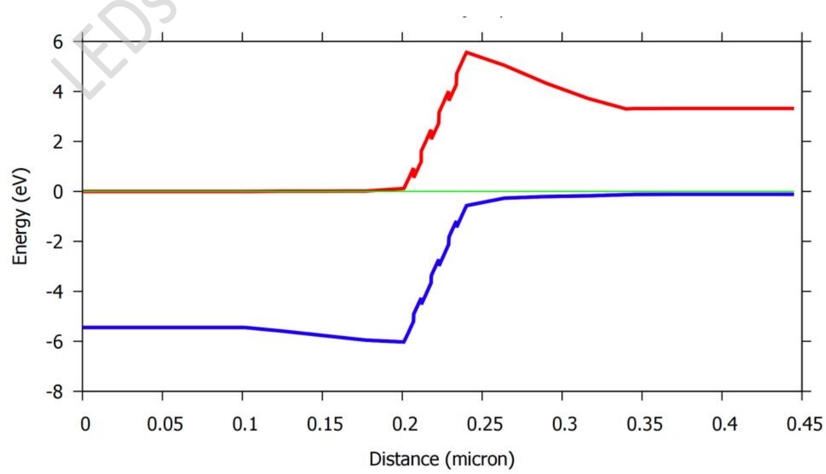

Fig. 5 Band diagram of ultraviolet LED representative struture

Quantum well Al composition/ultrathin AlN/GaN QW structure effects on IQE

The Al composition in quantum well plays an important role in determining the LED's electrical and optical properties because it has direct impact on the emission wavelength. As the Al composition in the QW layer increases, the bandgap widens, and the emission wavelength shifts to shorter wavelengths (higher energies). Therefore, by varying the Al composition in the QW layer, it is possible to tune the emission wavelength of the LED to specific UV wavelengths. The Al composition also affects the electron and hole confinement in the QW layer, which can affect the LED's efficiency and output power. When the Al composition in the QW layer is high, the electrons and holes are more tightly confined to the QW layer, which can lead to higher carrier densities and more efficient recombination. However, if the Al composition is too high, the electrons and holes may become trapped in defects or dislocations in the crystal structure, which can reduce the LED's efficiency and output power. In my project, I simulated various Al composition in the Al_xGaN QW from 60% Al to 82% Al while keeping the emission wavelength stay around 220 nm. The derived IQE, as shown in Fig. 6, changed as I expected. With the increasing Al composition, the internal quantum efficiency increases due to better carrier confinement.

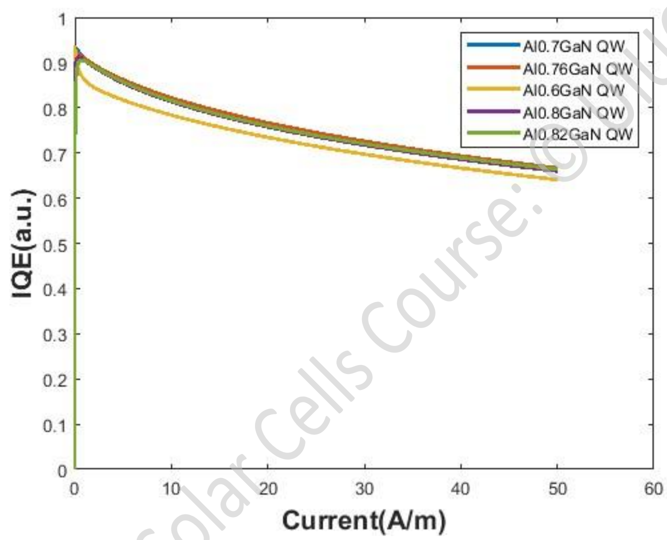

Fig. 6 The IQE of AlxGaN/AlN MQW UV LED for different Al compositions

In the way to increase the IQE of the UV LED, the greatest threat originates from nonradiative recombination in the active region. The internal electric fields induced by spontaneous and piezoelectric polarization in quantum wells tilt the conduction and valence bands, separate the electron and hole wave functions, and thus reduce their spatial overlap. It reduces the transition energy between the conduction and valence bands. Meanwhile, the radiative recombination probability also decreases. As a result, the quantum-confined Stark effect (QCSE) is observed for quantum wells with a very strong polarization effect. In order to against the spatial separation of wave functions in QCSE, I used an alternative MQW structure with binary ultrathin GaN/AlN, and the thickness of the GaN wells versus the AlN barriers was 1ML:4ML in order to keep the similar composition as the control $Al_{0.8}GaN$ sample. In terms of real growths, Wang et al. [8] fabricated similar electron-beam-pumped DUV light sources with ultrathin GaN/AlN MQWs by MOCVD and achieved a record output power of ~2.2 W operating at ~260 nm wavelength and Kobayashi et al. [9] arrived at a similar conclusion using an ultrathin MOVPE GaN(2ML)/AlN QWs with a remarkably improved photoluminescence (PL) intensity ratio of 50%. The mechanism behind the increased power and IQE is that both a higher energy barrier and spatial restrictions can expand the wavefunction overlap, enhance the quantum confinement effect, and improve the IQE by increasing the Al composition and adjusting the GaN well thickness, respectively. However, because it was hard to reproduce the growth condition of the ultrathin quantum well structure. I ended up getting an IQE even greatly lower than the normal MQW structure, as described in Fig. 7 below.

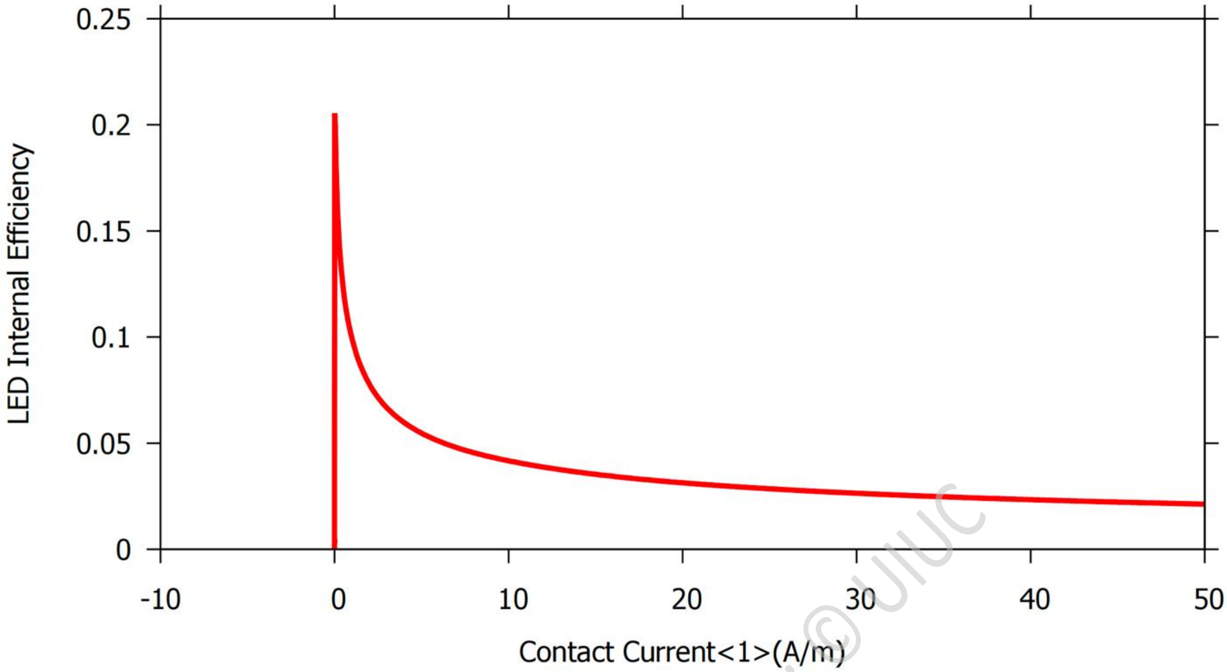

Fig.7 IQE of ultrathin GaN/AlN QW structure with GaN:AlN = 1ML:4ML

P-contact structure variation effects on IQE

p-type AlGaN layers with high electrical conductivity are essential for fabricating high-performance AlGaN-based DUV-LEDs. The high carrier concentration in the AlGaN layers not only produces a low resistance, but also guarantees great ohmic contact with the electrodes. Thus, the working voltage of DUV-LEDs is minimized, which results in lower thermal losses as well as a higher wall-plug efficiency and device reliability. Therefore, doping of AlGaN is one of the most important projects to date, but it is still accompanied by great challenges. One of the challenges is that the incorporation of dopant, Mg, into AlGaN is difficult to achieve. It has been theoretically confirmed that both the formation enthalpies of Mg_{Al} and Mg_{Ga} are positive and large in bulk AlGaN and increase with Al composition [10]. However, researchers have shown that AlGaN superlattice (SP) can be used to solve the problem. Mg acceptors in the AlGaN layer obtain electrons for ionization from the first miniband rather than the valence band, so that the activation energy is remarkably reduced. The minibands in the SL structure simultaneously facilitated hole transport.

Aside from the doping, light extraction efficiency is also a big concern for the IQE when designing a UV LED. For LEDs operating in the deep-ultraviolet (DUV) region ($\leqslant$ 280 nm), the LEE is generally <10% when compared with GaN-based LEDs emitting light with longer wavelengths. Here, three key factors are responsible for the limited LEE of DUV devices. First, the high Al component in AlGaN-based MQWs induces a large proportion of DUV light propagating parallel to the substrate surface with transverse magnetic polarization, and this partial light emitted from the sidewall cannot be effectively collected before it is absorbed by the active layers in the DUV device. Second, although the other part of the DUV light with transverse electric polarization can propagate along the c-axis for surface emission, the top p-GaN contact layer also absorbed considerable light owing to its relatively narrow bandgap. Finally, the total reflection at multiple interfaces further restricts LEE. In the simulation I mainly focused on solving the second problem, which is high absorption rate of p-GaN contact. Because DUV light is a short wavelength light with high photon energy, it is easily absorbed by GaN layer. Nevertheless, a p-GaN contact layer with a relatively small bandgap is commonly applied because of the difficulty in securing low-resistance p-AlGaN at high Al content. Typically, the transmittance at DUV wavelength is only ~5% for the DUV LED structure with a p-GaN contact layer, which can absorb majority of the DUV light emitted from the MQWs. Again, the short period super lattice (SL) can be used to solve the problem. Shatalov et al. [11] applied a p-type AlGaN/GaN short-period superlattice (SPSL) to replace p-GaN as the contact layer, and the transmittance dramatically increased to >60%, which resulted in an enhanced EQE of 10% for 275 nm LEDs. For my simulation, I replaced the 100 nm p-type GaN contact layer with repeated p-type Al_xGaN/undoped GaN contact layers, where x spans from 0 to 0.4. The IV, IQE and hole concentration results are shown in Fig. 8,9,10 below, respectively.

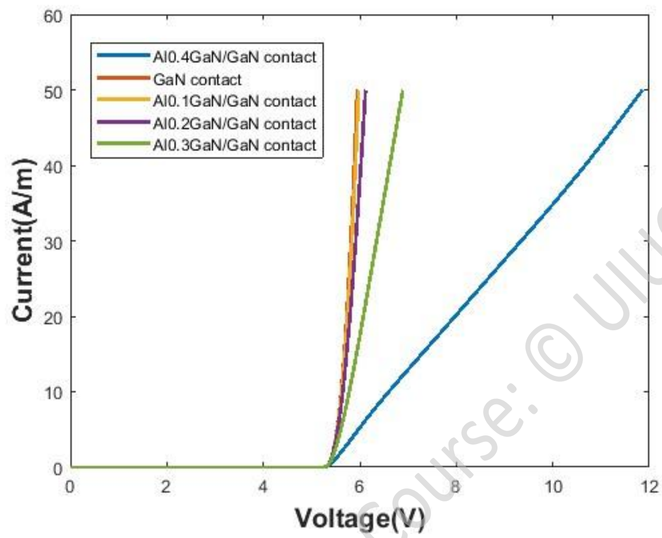

Fig. 8 IV of repeated Al_xGaN/GaN contact layers

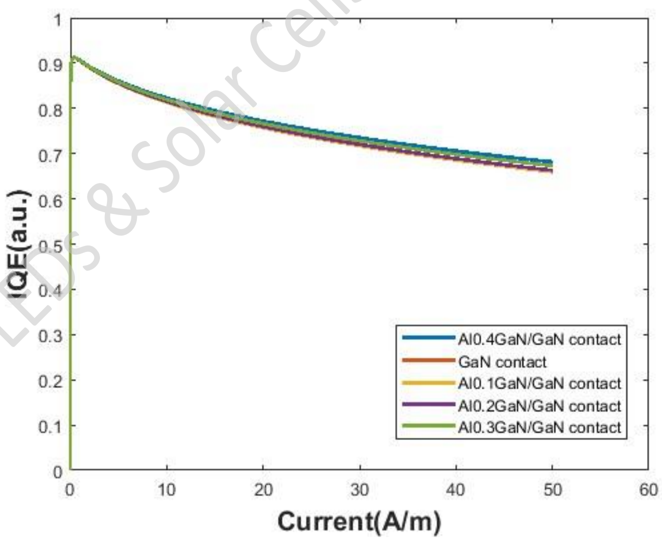

Fig. 9 IQE of repeated Al_xGaN/GaN contact layers

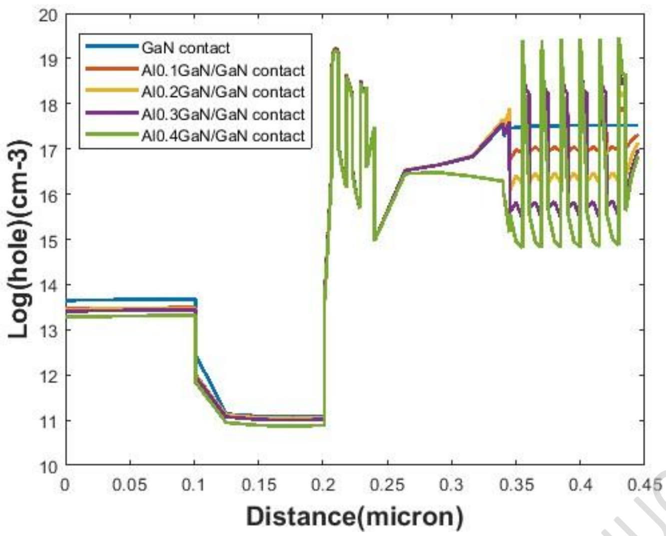

Fig. 10 Hole concentration of repeated Al_xGaN/GaN contact layers

From the figures we can see that though $Al_{0.4}GaN/GaN$ contact layer structure has slight advantage over the hole concentration and the internal quantum efficiency, it performs the worst in terms of the internal resistance due to its high Al concentration. On the other hand, though $Al_{0.3}GaN/GaN$ contact layer structure has slightly lower IQE and hole concentration, its great advantage in the internal resistance may make it a better choice in certain applications. Therefore we should make compromise among the parameters when we design the UVC LED.

Scaling effects on IQE

Micro-LEDs (µLEDs), with typical dimensions below 100 µm, have already attracted significant research attention in visible light applications, particularly in microdisplay and visible light communication. Generally, the size effect on micro LED's internal quantum efficiency (IQE) is that the IQE of the LED decreases as the size of the LED decreases. This effect is primarily due to the increased surface area-to-volume ratio of smaller LEDs, which can lead to increased surface recombination and non-radiative recombination.

As mentioned in the technical background session above, in LEDs, the IQE is a measure of the efficiency with which electrons and holes recombine and emit photons. As the size of the LED decreases, the amount of material available for recombination also decreases. At the same time, the surface area of the LED increases, which can lead to increased surface recombination. Surface recombination occurs when carriers recombine at the surface of the LED, rather than in the active region where the recombination produces light. Since surface recombination is a non-radiative process, it reduces the IQE of the LED.

In addition to surface recombination, smaller LEDs may also experience increased non-radiative recombination due to defects and impurities. Defects and impurities can act as recombination centers, effectively trapping electrons and holes and preventing them from recombining radiatively. In larger LEDs, the number of defects and impurities is spread out over a larger volume, which can reduce their impact on the overall IQE. However, in smaller LEDs, the concentration of defects and impurities is relatively high, which can lead to increased non-radiative recombination and a decrease in IQE.

However, DUV µLEDs can improve the efficiency owing to the relaxation of strain, enhancement of LEE, and mitigation of the severe current crowding effect. Therefore, the efficiency of DUV µLEDs won't necessarily decrease with scaling. For example, Yu et al. [12] investigated the size-dependent characteristics of DUV LEDs, achieving a 20% increase in EQE when the LED diameter is reduced from 300 μm to 20 μm. This revealed that smaller mesa areas can deliver higher LOP and uniform current spreading. The research group further verified that the EQE could be improved by inclining the chip sidewall, which is more effective in μLEDs with a 20–40 μm scale. Owing to their small areas and small junction capacitance, DUV μLEDs can be operated at high current densities and exhibit a high modulation bandwidth, which is an available light source for high-speed UV communication. Similarly, as my simulation of the scale effect on DUV LED IQE shown below, as the LED size L_1:L_2 scaled down from 120um:20um to 6um:1um, the IQE of the LEDs didn't strictly decrease with the decrease of the scale. Though the smallest scale, 6um:1um, did exhibit lowest IQE, other LEDs with small scales, such as the one with the size of 12um:2um, still have an IQE that is comparable to that of the largest scaled LED. Therefore, we can still achieve a decent internal quantum efficiency (~0.9) with a scale size of a few microns, which is the typical size for the DUV micro-LED to be used in environmental monitoring and medical equipment.

In addition, there are other methods can be used to mitigate the decrease of IQE as the decreased LED size, such as improving crystal quality and passivating the surface of the LED. However, because of the time limit of the project, I didn't have time to explore these thoughts.

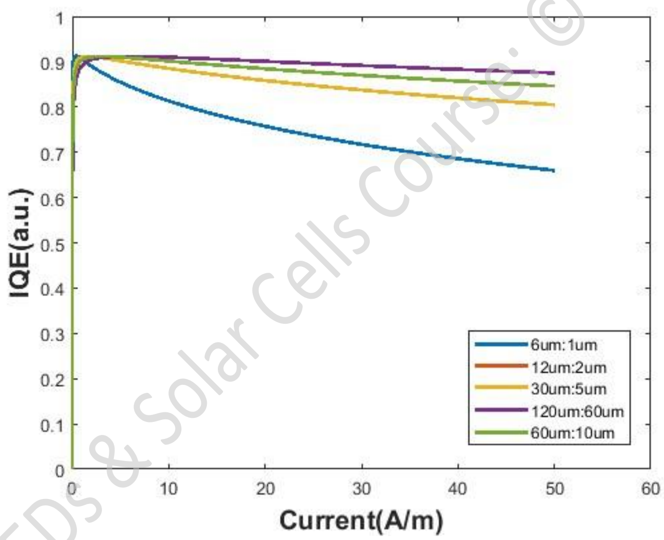

Fig. 11 Scale effect on IQE of DUV LED

Conclusion

AlGaN-based materials have exhibited considerable potential for fabricating ultraviolet (UV) light-emitting diodes (LEDs) owing to their direct, wide, and adjustable energy bandgap. AlGaN-based devices have extensive applicability owing to their stable physico-chemical properties. With decades of research effort, significant progress has been achieved in enhancing the working efficiency of AlGaN-based LEDs by optimizing the crystalline quality, doping efficiency, and device design. However, a DUV LED with high IQE is still hard to achieve because highly efficient p-type doping of AlGaN layers is difficult to achieve; the large difference in electron mobility and hole mobility in AlGaN-based materials increases the difficulty of fabricating devices with high injection efficiency for electrons and holes simultaneously; the quantum-confined Stark effect (QCSE) reduces the probability of radiative recombination between electrons and holes; the scale effect on LED increases the non-radiative recombination rate; and the extremely low light extraction efficiency further decreases the external quantum efficiency (EQE) of

AlGaN-based LEDs. In order to tackle those challenges and increase the efficiency of the DUV LED, in this project, I simulated several methods with calibrated layer composition and structure.

First, the Al composition in quantum well plays an important role in determining the LED efficiency because the Al composition affects the electron and hole confinement in the QW layer, which can affect the LED's efficiency and output power. According to my simulation, the IQE slightly increased as I increased the Al compostino from 0.6 to 0.82 for the Al_xGaN/AlN MQW structure. However, if the Al composition is too high, the electrons and holes may become trapped in defects or dislocations in the crystal structure, which can reduce the LED's efficiency. In addition, from the simulation we can see that the increase of the IQE became less significant as we further increased the Al composition. Therefore, we shouldn’t make the Al composition as high as possible if we want to design a good UVC LED. Instead, compromise must be made to other parameters.

Second, in order to against the spatial separation of wave functions in quantum-confined Stark effect (QCSE) and increase the LED efficiency, I used an alternative MQW structure with binary ultrathin GaN/AlN, and the thickness of the GaN wells versus the AlN barriers was 1ML:4ML in order to keep the similar composition as the control Al0.8GaN sample. According to the literature, this would give me a higher IQE because it increases the transition energy between the conduction and valence bands and the radiative recombination probability should also increase. However, because of the difficulty in reproducing the structure in Crosslight. The simulation went wrong, and I only ended up getting an IQE of ~20%.

Third, the doping efficiency of the p-type is the key factor for improving the internal quantum efficiency and decreasing the forward voltage because the high carrier concentration in the AlGaN layers not only produces a low resistance, but also guarantees great ohmic contact with the electrodes. Thus, the working voltage of DUV-LEDs is minimized, which results in lower thermal losses as well as a higher wall-plug efficiency and device reliability. In addition, light extraction efficiency is also a big concern for the IQE when designing a UV LED. For LEDs operating in the deep-ultraviolet (DUV) region ($\leqslant$ 280 nm), the LEE is generally <10% because the top p-GaN contact layer can absorb considerable light owing to its relatively narrow bandgap. Therefore, in my project, I design a p-tyep Al_xGaN/undoped GaN superlattice (SL) structure to replace the p-GaN contact. Though the IQE increased as the composition x changed from 0 to 0.4, the internal resistance got worse quickly as it changed from 0.3 to 0.4. Therefore, depending on the application, $Al_{0.4}GaN/GaN$ may not be the optimal choice.

Finally, because some applications such as sterilization of medical equipment and environmental monitoring require a DUV LED of a size in a few microns, the scaling effect on DUV LED must be studied. Unlike micro-LED that will have decreased IQE as the scale decreases due to increased surface recombination and non-radiative recombination originating from defects and impurities, the DUV µLEDs can improve the efficiency owing to the relaxation of strain, enhancement of LEE, and mitigation of the severe current crowding effect. In my project, I simulated my DUV LED structure with various scales of L_1:L_2. It turned out the IQE didn’t strictly decrease with the decreasing scale. Though small scales, such as L_1:L_2=12um:2um, still have smaller IQE compared to large scales, such as L_1:L_2=120um:20um. The decrease in IQE is already very small (within 3%).

There are also several ways to further improve my work. First, more simulations and studies can be done with the ultrathin GaN/AlN QW structure to check whether it can really give a boost on the IQE. Second, as for the scaling effect on IQE of the DUV LED, more parameters can be included to the structure during the simulation such as the surface recombination and surface passivation. Detailed simulation on Augur, radiative and Shockley-Read-Hall recombination can also be included to have a better understanding of the contributions from each component in the ABC model. Finally, the effect of donor doping level can also be considered because with the increase in Al composition, n-type dopant Si tends to relax from the donor state to an acceptor-like DX center, resulting in a dramatic increase in donor ionization energy thus a decrease in n-type doping level. Because the donor doping level is closely related to the internal resistance and IQE of the DUV LED, the topic is worth exploring if we want to further increase the LED efficiency.

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