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RESEARCH ARTICLE

Superior Optoelectronic Performance of N-Polar GaN LED to Ga-Polar Counterpart in the "Green Gap" Range

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ABSTRACT The low luminous efficiency of indium gallium nitride (InGaN) light-emitting diodes (LED) in the "green gap" range has been a long unsettled issue confounding the researchers. One of the main obstacles comes from the intrinsic polarization field in the incumbent Ga-polar LEDs (Ga-LEDs), where the polarization field will bend the energy band thus reducing the radiative recombination efficiency. The scenario will become different when we reverse the polarization field with the adoption of N-polar GaN, which should be a promising candidate to obtain LEDs with high luminous efficiency in the "green gap" range. In this study, the optical and electronic performances of InGaN LEDs in the "green gap" range with Ga- and N-polar have been numerically investigated. The results demonstrate that the light-output power of N-polar LED (N-LED) is ~1.69-fold higher than that of Ga-LED at a current density of 1250 A/cm^2, thus leading to a significantly improved internal quantum efficiency. Meanwhile, the turn-on voltage of N-LED is lowered by ~17.3% compared to that of Ga-LED. As revealed by the energy band diagram, the superior optoelectronic performance of N-LED is mainly attributed to the stronger carrier confinement in the active region and the lower carrier injection barriers. This study suggests the prospective realization of high luminous efficiency InGaN LEDs in the "green gap" range by the implementation of N-LEDs.

INDEX TERMS Green gap, light-emitting diodes, light-out power, N-polar, turn-on voltage.

I. INTRODUCTION

Gallium Nitride (GaN) and its related alloys are the important semiconductor materials in the application of light-emitting diodes (LEDs) due to the high luminous efficiency and the wide emission range in principle covering from ultraviolet to infrared [1]. In that the lack of centrosymmetry, wurtzite Ga-polar indium gallium nitride (InGaN) multiple quantum wells (MQWs) bear a strong polarization field with the magnitude of MV/cm [2]. Such a field will spatially separate the electrons and holes in the QWs and bend the energy band diagram, thus reducing the radiative recombination efficiency and exacerbating the carrier leakage from QWs, which is known as the quantum-confined Stark effect (QCSE) [3], [4], [5]. A large efficiency droop occurs in Ga-polar InGaN LEDs (Ga-LEDs) under high current injection and a large blue shift of emission wavelength appears, which are the dilemmas confronting the incumbent GaN-based light-emitting devices as most of the devices are fabricated on the Ga-polar GaN matrix. The efficiency droop will become even worse when the emission wavelength shifts to a longer side, e.g. >550 nm. This is because the high indium contents will cause a stronger

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piezoelectric polarization field and deteriorate the crystalline quality of InGaN, which is known as the "green gap" phenomenon [6]. Many efforts have been made to bridge the "green gap" [6], [7], [8], [9]. However, up to date, the external quantum efficiency (EQE) of red InGaN LEDs is still lower than 3% [10]. Recently, N-polar LED (N-LED) has been reported to be an effective candidate to break through the bottleneck faced by Ga-LED [10], [11], [12], [13]. The polarization field in N-LED is in a reverse direction compared to that of Ga-LED, thus having some intrinsic merits to suppress the efficiency droop effect and carrier leakage problem [14]. In addition, a higher indium and magnesium incorporation efficiency of N-polar GaN than that of Ga-polar GaN is also reported by researchers, revealing a potential to realize long wavelength InGaN LEDs with a high luminous efficiency [15], [16]. The lack of high quality N-polar GaN hinders the development of N-polar GaN-based devices. In the recent years, N-polar GaN with an atomic smooth surface and reduced defects grown by metal organic chemical vapor deposition (MOCVD) has been reported by researchers [17], [18], [19], [20], and the N-polar high electron mobility transistors (HEMTs), ultraviolet LEDs with superior performance have also been designed [21], [22], [23], [24], [25]. However, seldom experimental reports could be found for the investigation of N-polar red LEDs [10]. Moreover, as the growth conditions and the quality of epilayers are rather different for N-LED and Ga-LED (e.g. the chamber pressure, the V/III ratio, the initial growth condition, the defects in the expilayers, and so on), a meaningful experimental comparison between N-LED and Ga-LED remains challenging [4], [17], [26]. Some researchers reported the outperformed optoelectronic performance of N-LED than Ga-LED. However, the emission wavelengths are restricted in the blue emission regime, and more insight into the mechanisms have not been deeply discussed, e.g. the energy levels of both electron and hole in the MQWs regions which significantly affect the radiative recombination efficiency and carrier overflow [12], [14]. Therefore, a theoretical investigation for the N-LED in the "green gap" range should be necessary.

In this study, we numerically investigated the optical and electrical performance of Ga-LED and N-LED in the "green gap" range by the commercially available Crosslight APSYS software. A superior performance was demonstrated by N-LED to that of Ga-LED with enhanced internal quantum efficiency (IQE) and reduced turn-on voltage. According to the energy band diagram, the stronger carrier confinement in the QWs and the improved carrier injection efficiency should account for the transcendental performance of N-LED.

II. DEVICE STRUCTURE

The structure of Ga-LED and N-LED is depicted in Fig. 1(a). Five periods of MQWs [$In_{0.35}GaN$(3 nm)/$In_{0.02}GaN$(10 nm)] are sandwiched between a 3 μm-thick n-GaN (with an n-type doping concentration of 1×10^{18} cm^{-3}) and a 20 nm-thick p-$Al_{0.15}GaN$ (with a p-type doping concentration of 1×10^{18} cm^{-3}) electron blocking layer (EBL). The MQWs are undoped. Above the EBL, a 120 nm-thick p-GaN (with a p-type doping concentration of 5×10^{18} cm^{-3}) clads. The p- and n-contacts are Ohmic contacts with a dimension of 100 μm and 80 μm, respectively. The mesa dimension is 200 μm. According to the default setting of Crosslight APSYS, the width of the device is 1 m. The only difference for Ga-LED and N-LED is the direction of polarization field, which is along +c direction for Ga-LED while for N-LED is along –c. During the simulation, the Shockley–Read–Hall (SRH) lifetime within QWs is estimated to be 100 ns, similar to the reported values [27]. The Auger recombination coefficient and radiative recombination coefficient are set to be 1×10^{-34} cm^6/s and 2×10^{-11} cm^3/s, respectively [12]. The spontaneous and piezoelectic polarization are based on the method proposed by Fiorentini *et al.* [28]. Considering the partial compensation of polarization charge by fixed defects and other interface charges, we scale down the polarization charges with a factor of 0.3 for both samples. The self-consistent Poisson–Schrödinger and k·p models are employed for calculation of the MQW band structures [29].

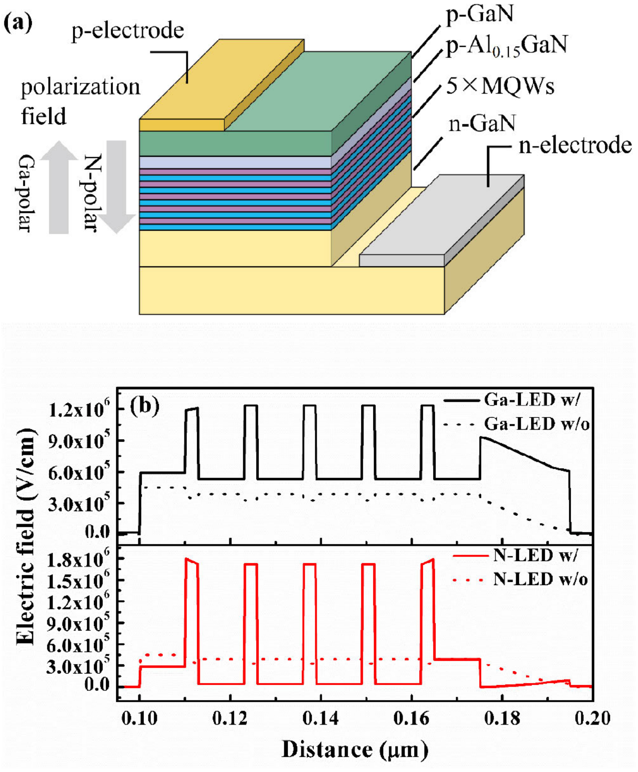

FIGURE 1. (a) The schematic structure of Ga-LED and N-LED. (b) The simulated built-in electric field in the MQWs regions with and without considering polarization effect of Ga-LED and N-LED.

III. RESULTS AND DISCUSSION

According to the default set of the APSYS software, only the total built-in electric field (i.e. the vector sum of p-n junction built-in field and the polarization field) could be extracted from the simulation. In order to evaluate the polarization field in the MQWs region, we simulated the built-in electric fields

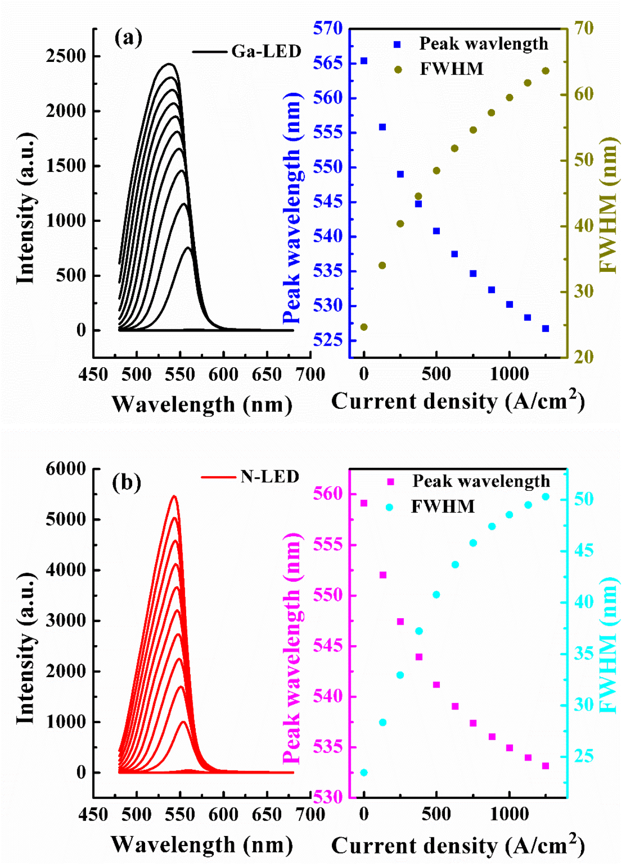

FIGURE 2. **(a, b) The emission spectra, peak wavelength and FWHM changing with current density of Ga-LED and N-LED, respectively.**

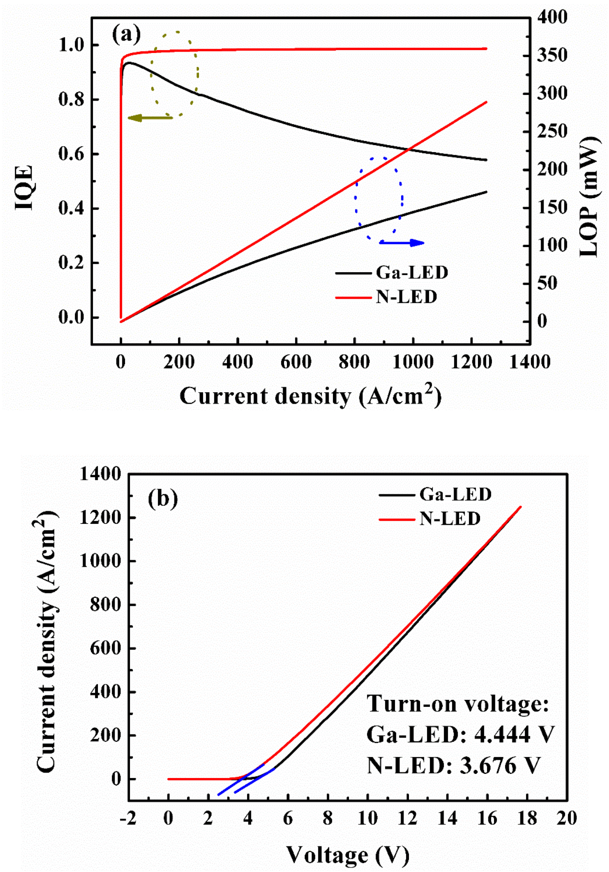

FIGURE 3. **(a) The IQE and LOP of Ga-LED and N-LED. (b) The I-V curves of Ga-LED and N-LED. The blue lines are the tangent lines to extract the turn-on voltages.**

with and without considering the polarization effect both for Ga-LED and N-LED at the equilibrium state (viz. zero bias). The results are delineated in Fig. 1(b). The fields tend to be a constant in the three middle QWs, therefore the polarization fields are estimated from this region, where the vector sums of spontaneous and piezoelectric polarization fields are 1.56 MV/cm and 1.39 MV/cm for Ga-LED and N-LED, respectively. As the simulation software is unable to decouple the spontaneous polarization field and piezoelectric polarization field separately, we evaluate the two polarization fields by using the equations suggested by Fiorentini *et al.* [28]. During the calculation, the dielectric constants of 9.5 for GaN [30] and 15.3 for InN [31] are used, and the lattice constants perpendicular to the c-axis of 3.189 angstrom for GaN and 3.545 angstrom for InN [32] are adopted. In conjunction with the Vegard's law and Gauss's law, the total polarization field in the QW is calculated to be 1.73 MV/cm, coinciding with the simulated results. The spontaneous polarization field and piezoelectric polarization field introduced by InGaN are -0.83 MV/cm and 1.56 MV/cm, respectively. With the concern of spontaneous polarization effect of GaN quantum barrier, the total spontaneous polarization field in QW is 0.17 MV/cm.

The emission spectra as well as the peak wavelength and full-width at half-maximum (FWHM) changing with injection current of Ga-LED and N-LED are presented in Figs. 2(a) and 2(b), respectively. Both of the two structures emit a light with a peak wavelength from ~560 nm to ~530 nm as the current increases, which locates in the "green gap" range. When the injection current increased to 1250 A/cm^2, the Ga-LED and N-LED all demonstrate a blue-shift of peak wavelength and an expansion of FWHM, indicating a screening effect of QCSE and a band filling effect [5]. However, N-LED exhibits a smaller blue-shift value (~26 nm) than that of Ga-LED of ~39 nm, indicating a more stable wavelength of N-LED under different currents. And the FWHM of N-LED is also a few nanometers narrower than that of Ga-LED, indicating an outperformed optical performance of N-LED.

The light-output power (LOP) and the IQE of Ga-LED and N-LED are shown in Fig. 3(a). The LOP of N-LED remains an almost constant impetus when the injection current increases to a large current density of 1250 A/cm^2, resulting in a nondrooping IQE (~98%). The high IQE and almost no efficiency droop in N-LED is in agreement with the results reported by other researchers [12], [33], indicating the suppression of carrier overflow, which will be discussed in detail in the following section. While the LOP of Ga-LED tends to a slower increment when the injection current increases to a high level, leading to a droop effect of IQE. The LOP of N-LED at 1250 A/cm^2 is ~1.69-fold higher than that of Ga-LED, indicating the superior optical performance of N-LED. The current-voltage (I-V) curves of Ga-LED and N-LED are represented in Fig. 3(b), where the blue lines are the extraction lines to estimate the turn-on voltage for each sample. As such, the turn-on voltage of N-LED is approximately 3.676 V, reduced ~17.3% from that of Ga-LED with ~4.444 V. The relatively high turn-on voltage for both structures should be partly attributed to the undoping of quantum barriers.

To reveal the mechanism behind the superior optoelectronic performance of N-LED, the energy band diagram is investigated for the two structures, as delineated in Fig. 4. Fig. 4(a) illustrates the energy band diagram at the equilibrium state, i.e. with zero bias. The reverse bending direction in MQWs of N-LED to that of Ga-LED indicates the reverse direction of polarization field in MQWs. The lift of the energy band of N-LED is due to the joint effect of polarization field and p-n junction built-in field. As the two kinds of electric field (i.e. polarization field and p-n junction built-in field) are along the same direction in N-LED, the energy band in the p-GaN side is elevated to a comparatively higher level than that in Ga-LED, where the p-n junction built-in field will partially compensate the polarization field. A representative band structure of QW2 is shown in the right side of Fig. 4(a), where the band levels and wavefunction of electrons and holes are clearly presented. The energy band diagrams for N-LED and Ga-LED under the injection current densities of 625 A/cm^2 (medium current density) and 1250 A/cm^2 (high current density) are illustrated in Figs. 4(b) and 4(c). Up to two electron energy levels and four hole energy levels exist in QW2-QW4 in N-LED both under medium and high current density injections, indicating an enhanced restriction of electrons and holes in the active region, which should improve the radiative recombination efficiency and suppress the carrier overflow. The right side of Figs. 4(b) and 4(c) represent a distinguishable description of the band structure of QW2 under medium and high currents respectively. As the droop effect will be more severe at high injection current, a detailed investigation from Fig. 4(c) is conducted. We find the barrier heights which the electrons on the ground state should surmount to escape out of the QW are higher in N-LED, with the values of 0.5875 eV, 0.5912 eV, 0.6187 eV, 0.6367 eV, and 0.6784 eV for QW1-QW5, respectively. While the barrier heights of Ga-LED for QW1-QW5 are 0.1462 eV, 0.1608 eV, 0.2176 eV, 0.2781 eV, and 0.3404 eV,

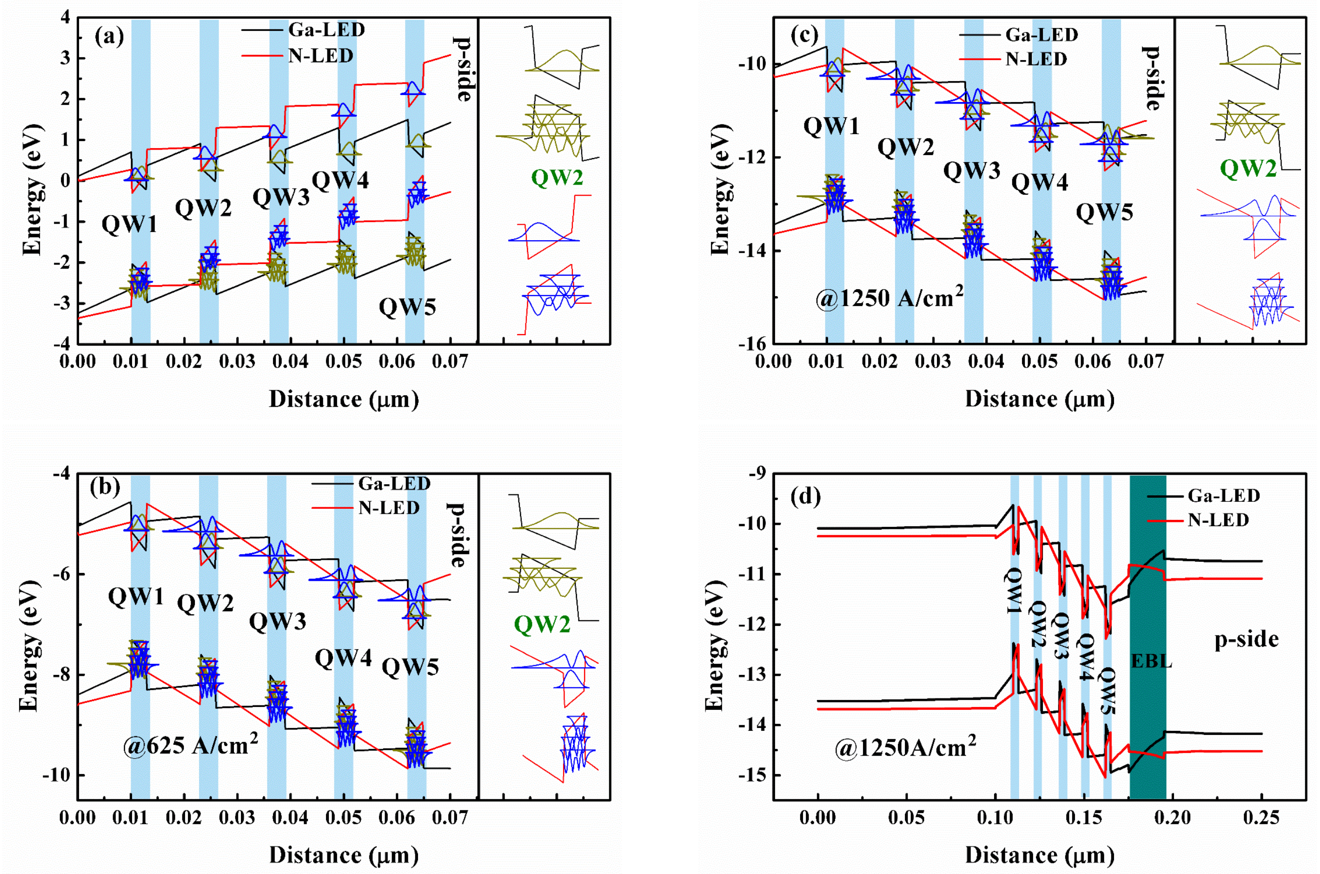

FIGURE 4. (a) The energy band diagram of QWs at equilibrium sate of Ga-LED and N-LED. The energy bands and the wavefuctions for electrons and holes are depicted in the figure with the dark yellow lines for Ga-LED and the blue lines for N-LED. right side: The typical band structure of Ga-LED and N-LED for QW2 at equilibrium state. (b) The energy band diagram of QWs under 625 A/cm^2 current injection of Ga-LED and N-LED. right side: The typical band structure of Ga-LED and N-LED for QW2 under 625 A/cm^2 current injection. (c) The energy band diagram of QWs under 1250 A/cm^2 current injection of Ga-LED and N-LED. right side: The typical band structure of Ga-LED and N-LED for QW2 under 1250 A/cm^2 current injection. (d) The energy band diagram from n-side to p-side under 1250 A/cm^2 current injection of Ga-LED and N-LED.

respectively, revealing a weakened restriction of electrons in Ga-LED. The barrier height of Ga-LED is more than half reduced, therefore the electrons tend to escape out of the MQWs region. Similar scenario could be found for holes in the valence band, where the barrier heights of N-LED in Fig. 4(c) for QW1-QW5 are 0.9058 eV, 0.7838 eV, 0.7394 eV, 0.7093 eV, and 0.7000 eV, respectively, while for Ga-LED are 0.6047 eV, 0.5465 eV, 0.4876 eV, 0.4304 eV, and 0.4147 eV, respectively. The barrier heights of N-LED are more than 60% higher than those of Ga-LED, indicating a stronger restriction for holes in N-LED. It should be noted, that the triangular potential of N-LED should lower the barrier a little due to the tunneling effect. However, as the deviations of barrier heights between N-LED and Ga-LED are extremely large, even considering the tunneling effect, it is reasonable to conclude that the N-LED preserves a higher barrier in the active region both for electrons and holes. A larger barrier height in the active region significantly improves the luminous efficiency of N-LED.

The lower turn-on voltage for N-LED should be attributed to the lower injection barrier for electrons in the n-side and holes in the p-side. From Fig. 4(d), the electron injection barriers in the n-side for N-LED and Ga-LED are 0.2563 eV, and 0.4595 eV, respectively. The injection barrier of N-LED is 44% lower than that of Ga-LED. It deviates a little with the results reported by Akyol *et al.*, in whose paper the electron barrier of N-LED is absent [12]. The hole injection barriers in the p-side of N-LED and Ga-LED are 0.1982 eV, and 0.8120 eV, respectively, ~76% lower in N-LED. As the injection barriers for electrons and holes of Ga-LED are sufficiently high, the forward voltage of Ga-LED is higher than that of N-LED.

IV. CONCLUSION

In conclusion, we investigated the optical and electrical performance of Ga- and N-LEDs in the "green gap" range. The N-LED demonstrates a higher LOP and an almost non-drooping IQE as well as a lower turn-on voltage than those of Ga-LED. The reversed polarization field induces an ultimate different energy band diagram for N-LED compared to Ga-LED. The stronger carrier restriction in the active region and the lowered carrier injection barriers in the n- and p-sides should account for the superior optoelectronic performance of N-LED. This study gives a deep insight into the mechanism of optical and electrical performance of N-LED in the "green gap" range, thus providing a promising means of bridging the "green gap".

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