

1 Hole transport assisted by the piezoelectric field in $\text{In}_{0.4}\text{Ga}_{0.6}\text{N}/\text{GaN}$ quantum wells
2 under electrical injection

3

4 Shuailong Zhang,^{1,2,a,b} Enyuan Xie,^{1,a} Tongxing Yan,^{3,a} Wei Yang,³ Johannes
5 Herrnsdorf,¹ Zheng Gong,^{1,c} Ian M. Watson,¹ Erdan Gu,^{1,2,d} Martin D. Dawson,¹ and
6 Xiaodong Hu^{3,d}

7

8 1. *Institute of Photonics, SUPA, University of Strathclyde, Glasgow G4*
9 *0NW, UK*

10 2. *Joint Laboratory of Advanced Optoelectronic Materials and Devices,*
11 *State Key Laboratory, Wuhan University of Technology, China and*
12 *Institute of Photonics, University of Strathclyde, Glasgow G4 0NW, UK*

13 3. *State Key Laboratory for Artificial Microstructure and Mesoscopic*
14 *Physics, School of Physics, Peking University, Beijing 100871, China*

15

16 a) *Shuailong Zhang, Enyuan Xie and Tongxing Yan contributed equally to this work.*

17 b) *Current address: School of Engineering, University of Glasgow, G12 8LT, United*
18 *Kingdom.*

19 c) *Current address: mLED Ltd., Glasgow G1 1XN, United Kingdom.*

20 d) *Email: erdan.gu@strath.ac.uk; huxd@pku.edu.cn*

21

22

23 ABSTRACT:

24

25 The authors observe the significant penetration of electrically injected holes through
26 InGaN/GaN quantum wells (QWs) with an indium mole fraction of 40%. This effect
27 and its current density dependence were analysed by studies on micro-pixel light-
28 emitting diodes, which allowed current densities to be varied over a wide range up to
29 $5 \text{ kA}/\text{cm}^2$. The systematic changes in electroluminescence spectra, are discussed in
30 the light of the piezoelectric field in the high-indium-content QWs and its screening
31 by the carriers. Simulations were also carried out to clarify the unusual hole transport
32 mechanism and the underlying physics in these high-indium QWs.

33

34

35

36

37

38

39

40

41

1 I. INTRODUCTION:

2 InGaN-based light-emitting diodes (LEDs) have the capability to generate
3 light across the whole visible spectrum, making them suitable light sources for a wide
4 range of applications such as solid-state lighting, signalling, displays, and medical
5 applications [1] [2]. The light emitting region in these LEDs is typically an
6 InGaN/GaN multi-quantum-well (MQW) structure where the indium composition of
7 the QWs determines the emission wavelength. However, as the indium content in the
8 InGaN alloy increases above 25%, the quantum efficiency of the LEDs significantly
9 drops, limiting the applications of InGaN LEDs with emission wavelengths longer
10 than 520 nm [3]. The poor quantum efficiency of high-indium content LEDs
11 compared to that of mature blue/green LEDs is mainly due to the strong strain-
12 induced piezoelectric field and the high dislocation/defect density in the LED
13 epitaxial structure [3]-[6].

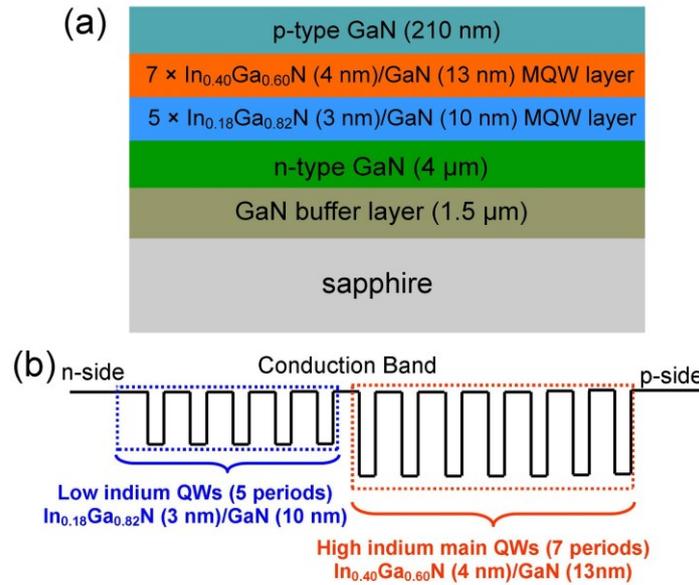
14 The carrier transport and distribution mechanism in mature blue/green InGaN
15 LEDs have been systematically studied before, which has been proved to have
16 significant influence on the properties of the devices [7]-[14]. However, there is very
17 little research on the carrier transport and distribution mechanism in InGaN LEDs
18 with indium mole-fractions over 30%. Due to the high-indium content in the active
19 region, such LEDs show many different electrical and optical properties compared
20 with low-indium blue/green InGaN LEDs [3] [15]. Additionally, improvements of the
21 quality of high-indium InGaN/GaN quantum wells (QWs) enabled important
22 demonstrations and applications of LEDs with long emission wavelengths for
23 phosphor-free white lighting, colour-conversion and displays [16]-[19]. Therefore, a
24 clear understanding of the carrier dynamics in high-indium InGaN LEDs can help to
25 optimize the LED epitaxial structure for better device performance and the
26 aforementioned applications.

27 In this work, we investigated the carrier transport and distribution in an LED
28 structure comprising 7 QWs with 40% indium content and 5 QWs with 18% indium
29 content. In particular, the electroluminescence (EL) of this LED was studied over a
30 wide current density range up to several kA/cm². This was enabled by fabricating so-
31 called “micro-LEDs”, i.e. LEDs with typical sizes of several tens of microns or less.
32 Due to a reduction in device self-heating and current crowding, micro-LEDs are able
33 to be driven at very high current densities with very high output power densities,
34 enabling many novel LED applications and the study of LED characteristics in a wide

1 current density range not accessible using conventional broad-area LEDs [20]-[23]. In
2 this work, it is found that a significant number of holes penetrates through the seven
3 repeat periods of high-indium-content QWs and recombines with electrons in the low-
4 indium-content QWs which are located at the n-side of the junction region.
5 Additionally, we present evidence that the fraction of holes penetrating through the
6 high-indium QWs is dependent on the current density. A finite element simulation
7 indicates that an important factor influencing the hole transport is piezoelectric field
8 which weakens the confining capability of QWs to holes. In this case, the screening of
9 piezoelectric field explains the observed current density dependence.

11 II. LED WAFER EPITAXIAL GROWTH AND DEVICE FABRICATION

12 The LED wafer used for micro-LED device fabrication was grown on a *c*-plane
13 sapphire substrate by metal organic chemical vapour deposition. Fig. 1 (a) shows the
14 epitaxial structure of the LED wafer, which consists of a 1.5 μm thick GaN buffer
15 layer, a 4 μm thick n-type GaN layer, a MQW region and a 210 nm thick p-GaN cap
16 layer. The MQW region contains a five-period $\text{In}_{0.18}\text{Ga}_{0.82}\text{N}$ (3 nm)/GaN (10 nm)
17 MQW layer emitting at 460 nm (“bottom QWs”), and a seven-period $\text{In}_{0.40}\text{Ga}_{0.60}\text{N}$ (4
18 nm)/GaN (13 nm) MQW layer emitting at 600 nm (“main QWs”). More details of the
19 LED wafer, including photoluminescence measurement, can be found in our previous
20 work [5]. Fig. 1 (b) shows a schematic diagram of the conduction energy band
21 without polarization field in the active region of the LED wafer material. The low-
22 indium-content blue QWs function as an electron reservoir for improving the radiative
23 efficiency of the main QWs [24] [25]. More importantly, the main QWs have very
24 high indium mole fraction, inducing 4.27% lattice mismatch between $\text{In}_{0.40}\text{Ga}_{0.60}\text{N}$
25 and GaN. This large lattice mismatch leads to strong compressive strain in the main
26 QWs, which can result in the generation of defects, dislocations and alloy non-
27 homogeneity [15]. Here, the bottom low indium-content blue QWs may play another
28 beneficial role in partial strain relaxation, thus functioning to optimize the strain
29 distribution and improve the crystal quality of the main QWs [26].

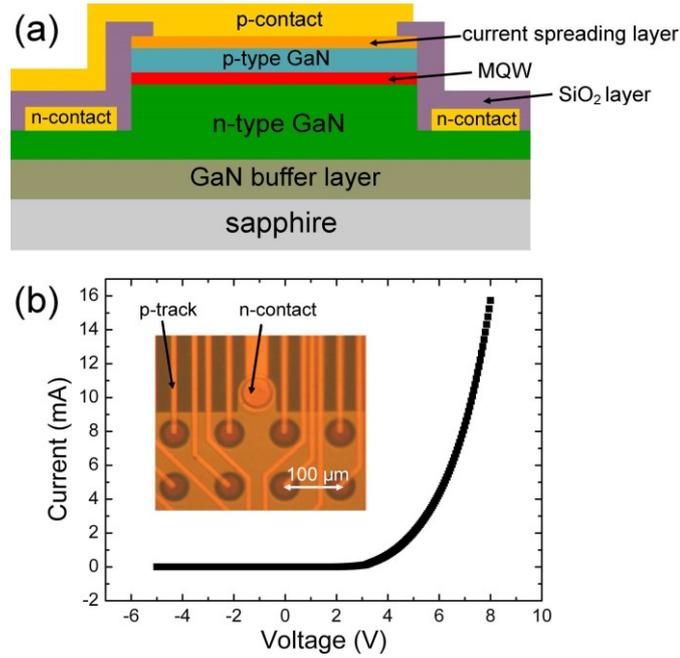


1

2 Figure 1: (a) Epitaxial structure of the dual-wavelength high-indium-content LED
 3 wafer; (b) schematic diagram of the conduction energy band of the active region of
 4 the LED wafer material (without polarisation effect).

5

6 The LED wafer was used to fabricate a 10 × 10 array of flip-chip micro-LEDs
 7 with 40 μm diameter on a 100 μm pitch. The mesa structure was first etched by Cl₂-
 8 based inductively coupled plasma down to the n-type GaN layer. After surface
 9 cleaning by a dilute HCl solution, a Ni/Au (10 nm/20 nm) metal bilayer was
 10 evaporated on the p-type GaN surface and thermally annealed in an air ambient at 500
 11 °C to form a semi-transparent metal contact on p-type GaN. The metallization on the
 12 n-type GaN was formed by depositing a Ti/Au (50 nm/200 nm) metal bilayer, which
 13 filled the area between each micro-LED and enabled an improved current spreading.
 14 Then, a 300 nm-thick SiO₂ layer was deposited by plasma-enhanced chemical vapour
 15 deposition to isolate each LED element. After selectively removing SiO₂ on top of
 16 each micro-LED, another Ti/Au metal bilayer was deposited on top of the oxidized
 17 Ni/Au bilayer as a reflector. This bilayer also connects each micro-LED pixel so as to
 18 individually address them. Fig. 2 (a) and (b) show a schematic cross-section and the
 19 current-voltage (I-V) characteristic of a typical micro-LED pixel from the array,
 20 respectively. A microscope image of a section of the array is also shown in the inset
 21 of Fig. 2 (b).



1

2 Figure 2: (a) Schematic cross-section and (b) I-V characteristic of a typical 40 μm
 3 diameter micro-LED pixel. The inset of (b) shows a microscope image of a section of
 4 the micro-LED array device.

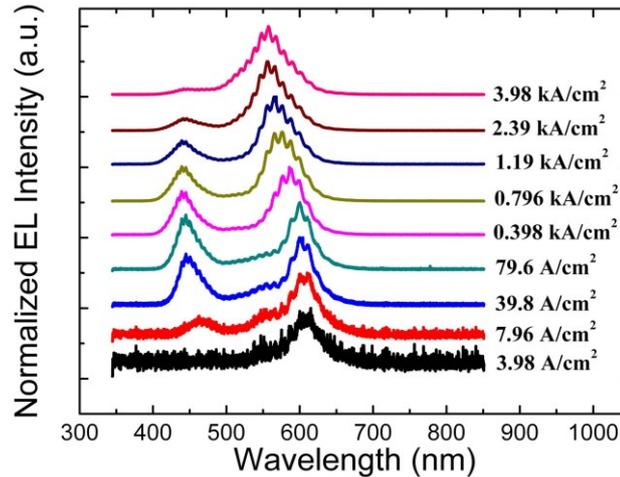
5

6 III. EXPERIMENTAL RESULTS AND DISCUSSIONS

7 The EL spectra of the micro-LED device were measured by a fibre-coupled
 8 CCD spectrometer (0.1 nm resolution, fibre with 0.22 NA) where the fibre was butt-
 9 coupled to the micro-LED. Fig. 3 shows the normalized EL spectra of a typical micro-
 10 LED pixel under different injection current densities, taken in pulsed operation (100
 11 μs pulse duration at 0.1 % duty cycle) to minimize thermal effects. Two dominant
 12 emission peaks can clearly be seen and are attributed to the main QWs (red-green
 13 emission) and the bottom QWs (blue emission). Both evolve differently as a function
 14 of injection current density.

15 The observation of a significant blue emission is surprising because holes have
 16 a high effective mass and a low mobility and therefore are a priori not expected to be
 17 injected into QWs deeper within the structure [8] [11] [27]-[29]. In previous work on
 18 low-indium-content LEDs, both direct observations, such as angle-resolved far-field
 19 measurement [8], and indirect indications based on EL spectra have shown that in
 20 these structures the QW closest to the p-side of the device has a much higher hole
 21 concentration than the other QWs [12]. It was also found that holes are more likely to
 22 transport into deep QWs with the increase of injection current [9]. However, as shown

1 in Fig. 3, the blue emissions in the spectra prove that holes can penetrate through the
 2 upper seven-period QWs and recombine in the bottom QWs. The spectra also indicate
 3 that such hole penetration and recombination vary with the injection current density.
 4 It is important to investigate and understand the physical mechanism responsible for
 5 such current-dependent deep hole injection in this LED structure.

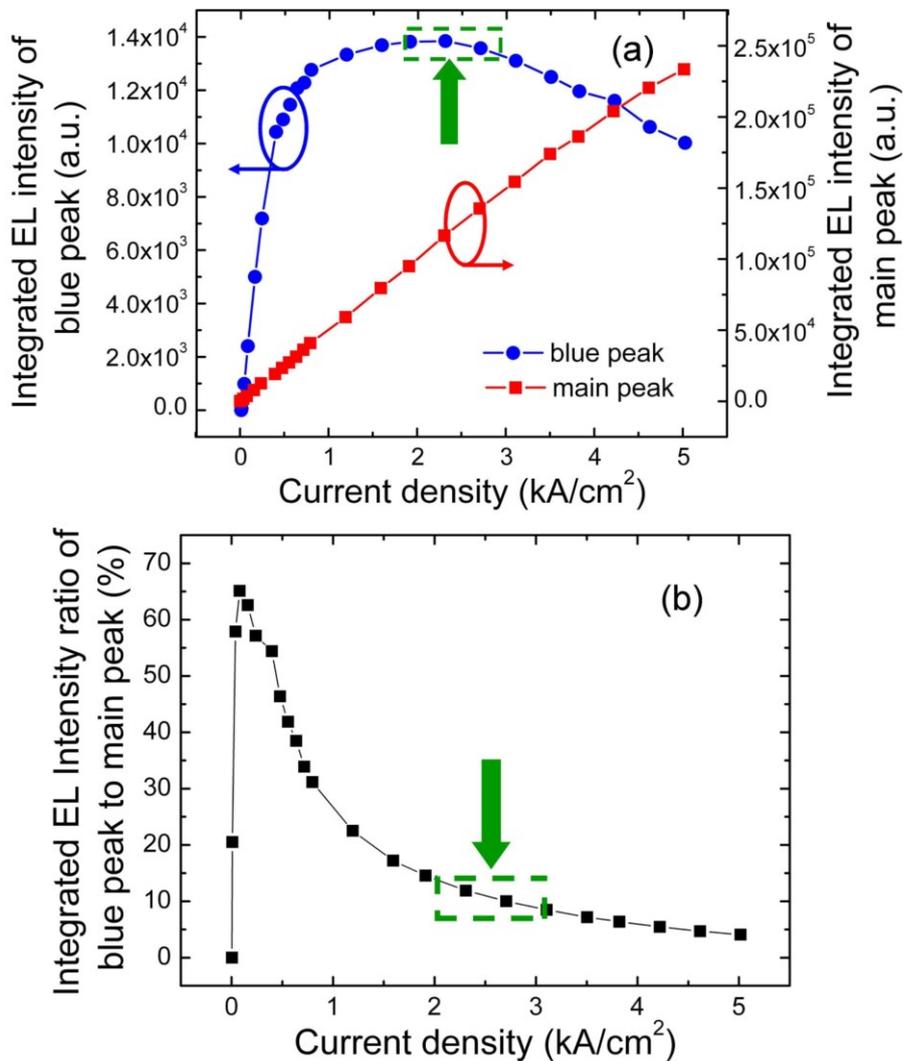


6
 7 Figure 3: Normalized EL spectra of a typical micro-LED pixel under different
 8 injection current densities. The micro-LED pixel is operated under pulsed conditions.
 9

10 We first discuss the EL spectra in more detail. In order to reduce the influence
 11 of detector noise, the measured spectra were fitted by two Gaussian peaks
 12 corresponding to main and blue emissions, respectively. Fig. 4 (a) shows the
 13 integrated EL intensities of the fitted peaks as a function of injection current density.
 14 The intensity of main peak steadily increases with increasing current density similar
 15 to that of conventional InGaN LEDs. In contrary, the intensity of the blue peak
 16 increases to a peak at around 2-2.3 kA/cm² and then drops with further increase of
 17 injection current density. Since electrons have a small effective mass and a high
 18 mobility, it can be assumed that the intensity of the blue peak reflects the distribution
 19 of holes in the device. From 0 to 1 kA/cm², there is an intense rise of emission
 20 intensity from bottom QWs, indicating that holes can be effectively injected into
 21 bottom QWs with the increase of current. From 1 to 3 kA/cm², the emission intensity
 22 from bottom QWs slightly increases to a peak at around 2-2.3 kA/cm² and then
 23 slightly decreases. After 3 kA/cm², the emission intensity from bottom QWs further
 24 drops with the increase of injection current density. Therefore, the hole transport is a
 25 current-dependent behaviour. The mechanism which enables the deep hole injection is

1 weakened with the increase of injection current, causing the drop of the EL emission
 2 intensity from the bottom QWs. Fig. 4 (b) shows the integrated EL intensity ratio of
 3 the blue peak to main peak. This ratio can be interpreted as a representation of the
 4 likelihood of holes to penetrate to the bottom QWs. It can be seen that holes have a
 5 significant likelihood to penetrate to the bottom QWs at low injection current
 6 densities while at high injection current densities holes are more likely to be trapped
 7 in main QWs. Additionally, above 3 kA/cm² the intensity ratio is stagnant between
 8 5% and 10%, whereas below 3 kA/cm² it varies strongly and a sharp drop of the
 9 intensity ratio can be clearly viewed.

10



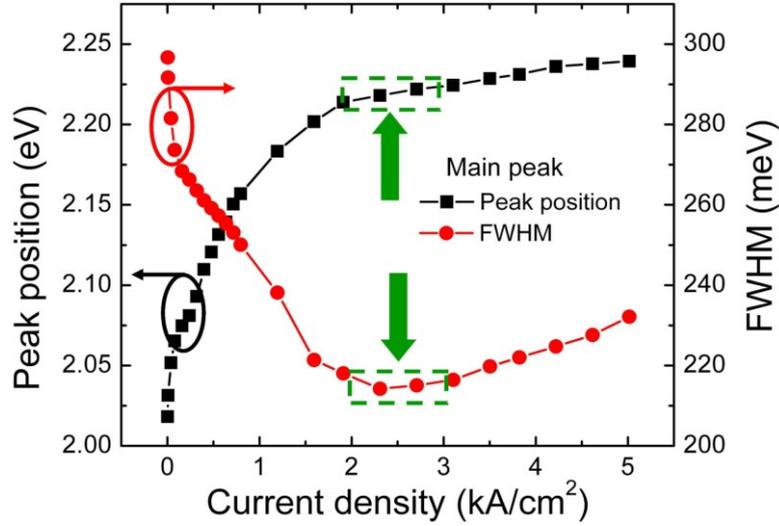
11

12 Figure 4: (a) Integrated EL intensity of the fitted two peaks (blue peak and main peak)
 13 from a typical micro-LED pixel under different injection current densities; (b)
 14 integrated EL intensity ratio of blue peak to main peak. The micro-LED pixel is
 15 operated under pulsed conditions.

1 We now explore the physical mechanisms controlling the hole distributions in
2 the QWs with different indium-contents. In the device discussed here, the
3 piezoelectric field in the main QWs has an important influence on the device
4 performance and is also a likely reason for the hole penetration [15]. In general, the
5 strong piezoelectric field and the current-dependent screening of the piezoelectric
6 field have a big influence on the band structure of QWs and thus the carrier dynamics
7 [15], [30]. In other words, the piezoelectric polarization due to lattice mismatch
8 induces a build-in electric field in the polar QW, known as the piezoelectric field.
9 This piezoelectric field can be screened by the injection carriers, which has a big
10 influence on the band structure of QWs and thus the carrier dynamics [5]. The
11 influence of the piezoelectric effect can be seen in the spectra shown in Fig. 3. At low
12 current densities the main QW emission peak occurs at the target wavelength of
13 600 nm. However, with the increase of current density, it blue-shifts to 550 nm which
14 is mainly due to two reasons, i.e. the screening of piezoelectric field (also known as
15 the screening of quantum confined Stark effect) and the band-filling effect [5],[31]-
16 [34]. However, the screening of piezoelectric field induces the narrowing of the
17 emission spectra due to the flat energy band and enhanced overlap of electron and
18 hole wave functions [35],[36]. While the band-filling effect induces the broadening of
19 the emission spectra [37]. Shown in Fig. 5 are the corresponding peak position and
20 full width at half maximum (FWHM) of the main peak extracted from the Gaussian fit.
21 It can be seen that, in the current density range from 0 to 3 kA/cm², there is a sharp
22 blue-shift (about 50 nm) of the peak position accompanied by a narrowing of the
23 FWHM. This indicates that, in this current density range, the blue-shift of the main
24 emission peak is dominated by the screening effect of the piezoelectric field by
25 injection carriers. Above 3 kA/cm², the FWHM increases associated with a slight
26 blue-shift of the peak position. In this regime, band-filling is likely the main driver for
27 the broadening of FWHM and the slight blue-shift. This interpretation is in good
28 agreement with our previous simulation results as the piezoelectric field is mostly
29 screened above 3 kA/cm² [5]. Therefore, the dominant factor determining the spectral
30 behaviour changes at a current density regime of 2-3 kA/cm², as indicated by the
31 green arrow and dashed box in Fig. 5. Interestingly, this current density regime also
32 matches very well with the current density regime highlighted by the green arrow and
33 dashed box in Fig. 4 (a) and (b), where the emission intensity of blue QWs reaches its
34 maximum value and the sharp drop of the integrated EL ratio stops. This coincidence

1 is an indication that the hole penetration below 3 kA/cm^2 is dominated by the
 2 piezoelectric field in the QWs.

3



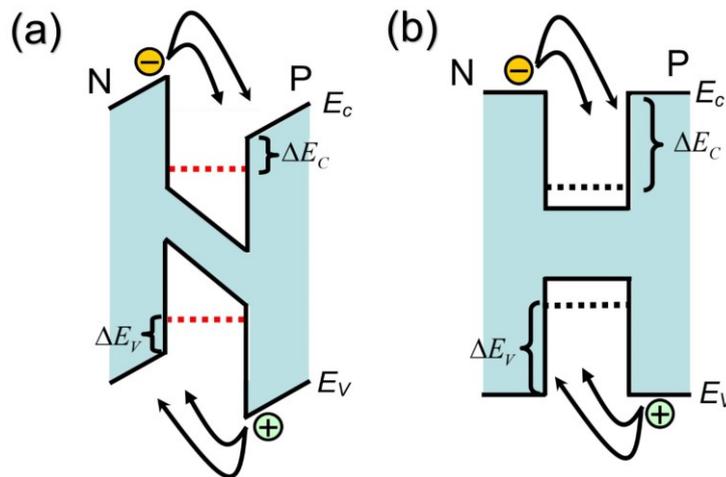
4

5 Figure 5: Peak position and corresponded FWHM of the main emission peak of a
 6 micro-LED pixel as a function of pulsed operating current.

7

8 This phenomenon can be interpreted as follows. A strong piezoelectric field
 9 severely tilts the band structure of QWs, decreasing the effective width of QW and
 10 subsequently leading to a strong flyover of carriers across the QW and a decrease of
 11 carrier capture rate of the QWs [15], [30]. Additionally, the ground state energy of
 12 electrons or holes in the narrow and tilted well is higher than that in the wider and
 13 standard well [15], [38], thus increasing the carrier escape rate. Also, the reduced
 14 overlap of hole and electron wave functions in a QW with piezoelectric field [7]
 15 results in a longer carrier lifetime and thus increases the chance of carrier escape. The
 16 schematics shown in Fig. 6 (a) and (b) illustrate these relevant factors on the carrier
 17 capture process and the energy state in a QW with and without piezoelectric field. As
 18 shown, the piezoelectric field can promote the transport of holes into deeper QWs
 19 while the screening of piezoelectric field can increase the confining capability of QWs,
 20 suppressing the transport of holes. It is probably for this reason that the emission from
 21 bottom QWs increases to a peak at around $2\text{-}2.3 \text{ kA/cm}^2$ and decreases at higher
 22 current densities. Additionally, the sharp drop of integrated intensity ratio shown in
 23 Fig. 4 (b) appears in the current density regime (before 3 kA/cm^2) where there is a
 24 strong screening of piezoelectric field ongoing and the stagnant of integrated intensity
 25 ratio appears in the current density regime (after 3 kA/cm^2) where the piezoelectric

1 field is severely minimized. In Fig.4, when the current increases in a range from 0 to
 2 0.079 kA/cm², the light intensity of bottom quantum wells increases relatively more
 3 significant than the light intensity of main quantum wells, inducing an increase of the
 4 ratio. This phenomenon has not been fully understood and is still under investigation.
 5 A possible reason is that the piezoelectric field in the bottom quantum wells is smaller
 6 than that in the main quantum wells. The smaller piezoelectric field in the bottom
 7 quantum wells is due to their lower indium mole fraction and corresponding smaller
 8 distribution of compressive strain. Details of the smaller piezoelectric field in bottom
 9 quantum wells, including experimental and simulation results, can be found in our
 10 previous work [5]. Therefore, the screening effect of carriers to piezoelectric field is
 11 relatively stronger than that in the main quantum wells under low injection current
 12 density and the light intensity of bottom quantum wells may increase relatively more
 13 significant than the light intensity of main quantum wells, inducing the increase of the
 14 ratio at low injection current density.



15
 16 Figure 6: Carrier capture process and schematic band diagram of an InGaN/GaN QW
 17 (a) with and (b) without piezoelectric field. Since the LED wafer was grown on *c*-
 18 plane sapphire substrate and the compressive strain exists in the QW (InGaN on top of
 19 GaN), the direction of piezoelectric field is from right hand side (P-GaN side) to left
 20 hand side (N-GaN side).

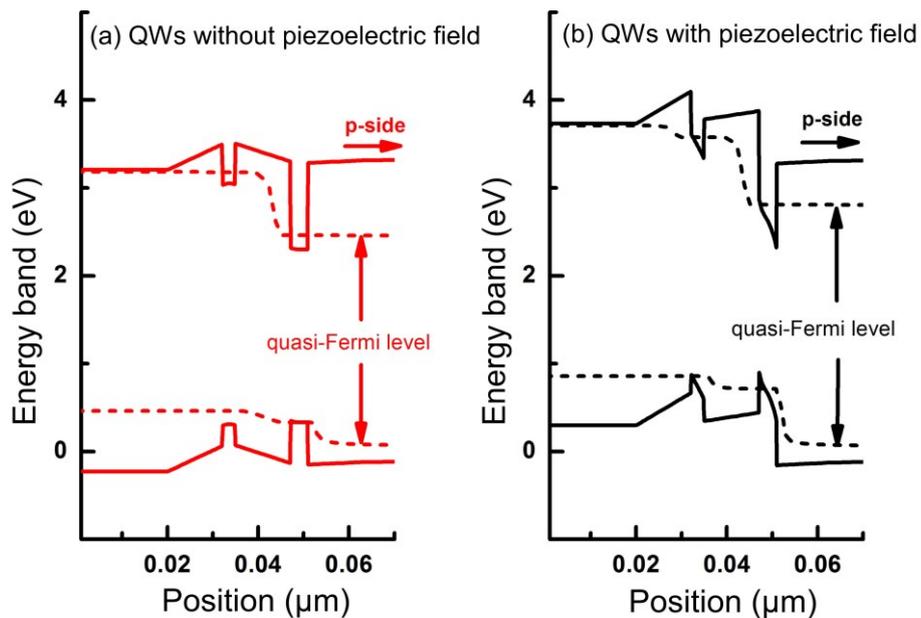
21
 22 In order to provide further insight on the influence of the piezoelectric field on
 23 hole transport mechanism in this dual-wavelength LED, simulations were carried out
 24 based on an advanced self-consistent k.p model embedded in a commercial simulation
 25 software APSYS [39]-[41]. This software couples Poisson equation, Schrödinger

1 equation in quantum well (by 6×6 band k.p theory for valence band and 2×2 effective
2 mass approximation for conduction band [41]), electron and hole current continuity
3 equation and LED ray-tracing equation. All equations were numerically solved
4 simultaneously by finite difference scheme with no-prior settings. More details of the
5 self-consistent k.p model and the simulation method can be found elsewhere [42]-[46].
6 The simulation in this work was based on the LED structure described in Section II,
7 except that a simple two set QWs were adopted: a low-indium-content ($\text{In}_{0.18}\text{Ga}_{0.82}\text{N}$)
8 QW layer (3 nm)/GaN (10 nm) and a high-indium-content ($\text{In}_{0.40}\text{Ga}_{0.60}\text{N}$) QW layer (4
9 nm)/GaN (13 nm). This simplification gives rapid convergence for simulation with
10 reasonable computation time, and at the same time does not hinder to reveal the
11 physical mechanism of our dual-wavelength LED structure. To demonstrate the
12 influence of piezoelectric field and the screening of piezoelectric field, two simulation
13 runs were performed: one with interface charge, which is automatically set by the
14 software according to indium composition; another one without interface charge,
15 which is manually set to zero. The simulation run with interface charge was used to
16 represent the practical case where there is a strong piezoelectric field existing in the
17 high-indium-content QW; while the simulation run without interface charge was used
18 to represent an ideal case that the piezoelectric field is screened. In this way, the
19 comparison of the QW with and without piezoelectric field can be made [47] [48]. It
20 is worth noting that the setting of interface charge in the simulation is equivalent to
21 that of piezoelectric field or polarization dipole moment [49]. 50% interface charge
22 (0.5 screening ratio) were adopted in the simulation run with interface charge due to a
23 weaker built-in polarization found in actual experiments [50],[51], which in our case
24 gives an interface charge density of $1.5\times 10^{13}/\text{cm}^2$ for the high-indium-content QW.
25 This screening ratio only represents the screening of doping and defects to
26 piezoelectric field [52]. All other material parameters used are from literature [53] and
27 were kept the same for the two runs.

28 Fig. 7 shows the energy band diagrams and quasi-Fermi levels of the QWs
29 with and without piezoelectric field. The injection current density is $500 \text{ A}/\text{cm}^2$. As
30 shown in Fig. 7 (a), in the valence band of the QWs without piezoelectric field, the
31 quasi-Fermi level is well above the band edge of the low-indium-content QW, which
32 indicates that very few holes can be injected into this QW. In contrast, in the valence
33 band of the QWs with piezoelectric field (Fig. 7 (b)), the quasi-Fermi level overlaps
34 the band edge of the low-indium-content QW, which indicates that holes can be

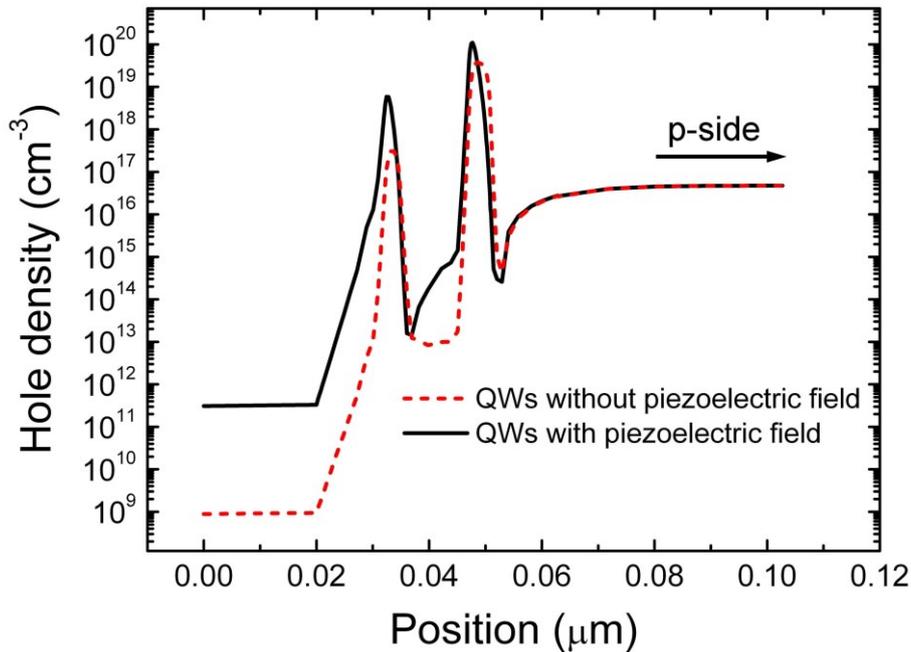
1 injected into this QW. In Fig. 7 (b), the band bending of p-side does not arise
 2 significantly nearby the interface between p-side and QW, which is mainly due to two
 3 reasons. Firstly, Fig. 7 (b) is plotted at an injection current density of 500 A/cm^2 ,
 4 applying such injection current density associated with high bias would flatten the
 5 band structure. Secondly, our structure does not have an AlGaIn electron blocking
 6 layer. Therefore, the piezoelectric polarization mismatch between the QW and p-type
 7 GaN is small. Fig. 8 shows the hole density of the QWs with and without
 8 piezoelectric field under an injection current density of 500 A/cm^2 . As shown, the
 9 hole density in the low-indium-content QW with piezoelectric field is an order of
 10 magnitude higher than that without piezoelectric field. In addition, the hole density
 11 ratio of low-indium-content QW to high-indium-content QW increases substantially
 12 when the piezoelectric field is applied. These simulation results match up well with
 13 the experimental results and prove that the piezoelectric field promotes the
 14 penetration of holes into deeper QWs. For QW with different Indium composition, the
 15 piezoelectric field and the screening effect of carriers also exist. Therefore, the reason
 16 of the hole penetration discussed in this work should play an role as well. However,
 17 the intensity of piezoelectric field and its screening by carriers in the QW varies
 18 strongly with different Indium composition. Our results show what happens in an
 19 extreme case of high indium composition and the exact dependence of the effect on
 20 the indium composition will be studied in the future.

21



22

1 Figure 7: Energy band diagrams of QWs (a) without piezoelectric field and (b) with
 2 piezoelectric field under an injection current density of 500 A/cm^2 .
 3



4
 5 Figure 8: Hole concentrations of the QWs with and without piezoelectric field under
 6 an injection current density of 500 A/cm^2 .
 7

8 IV. CONCLUSION:

9 In summary, we have investigated the effect of hole penetration through a number
 10 of high-indium-content QWs in an InGaN micro-LED. It is demonstrated that the hole
 11 transport mechanism in this structure depends on the current density and coincides
 12 with screening of the built-in piezoelectric field. Studies on micro-LEDs allowed the
 13 current density to be varied over a wide range, up to 5 kA/cm^2 . Based on the EL
 14 spectra, it is discussed how the piezoelectric field and its screening can indeed explain
 15 the observed behaviour of the device. Furthermore, this view is underpinned by
 16 simulation results which show that the piezoelectric field can increase the capability
 17 of hole transport into deeper QWs. Therefore, by investigating the carrier transport
 18 and distribution, this research provides insight into the piezoelectric field related
 19 mechanism underlying the current-dependent EL spectra observed in the high-indium-
 20 content InGaN micro-LED device.

21

22

1 ACKNOWLEDGMENTS

2 This work was supported by the Engineering and Physical Sciences Research
3 Council through HYPIX Project under Grant EP/F05999X/1 and Ultra-parallel
4 Visible Light Communications Project under Grant UP-VLC EP/K00042X/1.

5

6 REFERENCE

7

- 8 [1] E. F. Schubert and J. K. Kim, "Solid-State Light Sources Getting Smart",
9 *Science*, **308**, 1274 (2005).
- 10 [2] S. Pimputkar, J. S. Speck, S. P. DenBaars, and S. Nakamura, "Prospects for
11 LED lighting", *Nat. Photon.*, **3**, 180 (2009).
- 12 [3] T. Mukai, M. Yamada, and S. Nakamura, "Characteristics of InGaN-based
13 UV/blue/green/amber/red light-emitting diodes", *Jap. J. Appl. Phys.*, **38**, 3976,
14 (1999).
- 15 [4] J.-I. Hwang, R. Hashimoto, S. Saito, and S. Nunoue, "Development of InGaN-
16 based red LED grown on (0001) polar surface", *Appl. Phys. Exp.*, **7**, 071003
17 (2014).
- 18 [5] Z. Gong, N. Y. Liu, Y. B. Tao, D. Massoubre, E. Y. Xie, X. D. Hu, Z. Z. Chen,
19 G. Y. Zhang, Y. B. Pan, M. S. Hao, I. M. Watson, E. Gu, and M. D. Dawson,
20 "Electrical, spectral and optical performance of yellow–green and amber
21 micro-pixelated InGaN light-emitting diodes", *Semicond. Sci. Technol.*, **27**,
22 015003 (2012).
- 23 [6] H.-S. Chen, C.-F. Lu, D.-M. Yeh, C.-F. Huang, J.-J. Huang, and C.-C. Yang,
24 "Orange–red light-emitting diodes based on a prestrained InGaN–GaN
25 quantum-well epitaxy structure", *IEEE Photon. Technol. Lett.*, **18**, 2269
26 (2006).
- 27 [7] R. Charash, P. P. Maaskant, L. Lewis, C. McAleese, M. J. Kappers, C. J.
28 Humphreys, and B. Corbett, "Carrier distribution in InGaN/GaN tricolor
29 multiple quantum well light emitting diodes", *Appl. Phys. Lett.*, **95**, 151103
30 (2009).
- 31 [8] A. I. David, M. J. Grundmann, J. F. Kaeding, N. F. Gardner, T. G. Mihopoulos,
32 and M. R. Krames, "Carrier distribution in (0001)InGaN / GaN multiple
33 quantum well light-emitting diodes," *Appl. Phys. Lett.*, **92**, 053502 (2008).
- 34 [9] M. Meneghini, S. Vaccari, A. Garbujo, N. Trivellin, D. Zhu, C. J. Humphreys,
35 M. Calciati, M. Goano, F. Bertazzi, G. Ghione, E. Bellotti, G. Meneghesso,
36 and E. Zanoni, "Electroluminescence Analysis and Simulation of the Effects
37 of Injection and Temperature on Carrier Distribution in InGaN-Based Light-
38 Emitting Diodes with Color-Coded Quantum Wells", *Jap. J. Appl. Phys.*, **52**,
39 08JG09 (2013).
- 40 [10] T. S. Kim, B. J. Ahn, Y. Dong, K. N. Park, J. G. Lee, Y. Moon, H. K. Yuh, S.
41 C. Choi, J. H. Lee, S. K. Hong, and J. H. Song, "Well-to-well non-uniformity
42 in InGaN/GaN multiple quantum wells characterized by capacitance-voltage
43 measurement with additional laser illumination", *Appl. Phys. Lett.*, **100**,
44 071910 (2012).
- 45 [11] J. Cho, E. F. Schubert, and J. K. Kim, "Efficiency droop in light-emitting
46 diodes: Challenges and countermeasures", *Laser Photon. Rev.*, **7**, 408 (2013).

- 1 [12] J. P. Liu, J. H. Ryou, R. D. Dupuis, J. Han, G. D. Shen, and H. B. Wang,
2 "Barrier effect on hole transport and carrier distribution in InGaN / GaN
3 multiple quantum well visible light-emitting diodes", *Appl. Phys. Lett.*, **93**,
4 021102 (2008).
- 5 [13] J.-Y. Zhang, L.-E. Cai, B.-P. Zhang, X.-L. Hu, F. Jiang, J.-Z. Yu, Q.-M. Wang,
6 "Efficient hole transport in asymmetric coupled InGaN multiple quantum
7 wells", *Appl. Phys. Lett.*, **95**, 161110 (2009).
- 8 [14] Z. Zheng, Z. Chen, Y. Chen, H. Wu, S. Huang, B. Fan, Z. Wu, G. Wang and H.
9 Jiang, "Improved carrier injection and efficiency droop in InGaN/GaN light-
10 emitting diodes with step-stage multiple-quantum-well structure and hole-
11 blocking barriers", *Appl. Phys. Lett.*, **102**, 241108 (2013).
- 12 [15] E. F. Schubert. Light-emitting diodes. Cambridge University Press, second
13 edition, 2008.
- 14 [16] M. Yamada, Y. Narukawa, and T. Mukai, "Phosphor Free High-Luminous-
15 Efficiency White Light-Emitting Diodes Composed of InGaN Multi-Quantum
16 Well", *Jap. J. Appl. Phys.*, **41**, 246 (2002).
- 17 [17] Y. J. Hong, C.-H. Lee, A. Yoon, M. Kim, H.-K. Seong, H. J. Chung, C. Sone,
18 Y. J. Park, and G.-C. Yi, "Visible-Color-Tunable Light-Emitting Diodes", *Adv.*
19 *Mater.*, **23**, 3284 (2011).
- 20 [18] B. Damilano, H. K.-Chauveau, E. Frayssinet, J. Brault, S. Hussain, K. Lekhal,
21 P. Vennegues, P. D. Mierry, and J. Massies, "Metal Organic Vapor Phase
22 Epitaxy of Monolithic Two-Color Light-Emitting Diodes Using an InGaN-
23 Based Light Converter", *Appl. Phys. Exp.*, **6**, 092105 (2013).
- 24 [19] S. Zhang, Z. Gong, J. J. D. McKendry, S. Watson, A. Cogman, E. Xie, P. Tian,
25 E. Gu, Z. Chen, G. Zhang, A. E. Kelly, R. K. Henderson, M. D. Dawson,
26 "CMOS-Controlled Color-Tunable Smart Display", *IEEE Photon. J.*, **4**, 1639
27 (2012).
- 28 [20] Z. Y. Fan, J. Y. Lin, and H. X. Jiang, "III-nitride micro-emitter arrays:
29 development and applications", *J. Phys. D: Appl. Phys.*, **41**, 094001 (2008).
- 30 [21] H. X. Jiang and J. Y. Lin, "Nitride micro-LEDs and beyond - a decade
31 progress review", *Opt. Exp.*, **21**, A475 (2013).
- 32 [22] Z. Gong, S. Jin, Y. Chen, J. McKendry, D. Massoubre, I. M. Watson, E. Gu,
33 and M. D. Dawson, "Size-dependent light output, spectral shift, and self-
34 heating of 400 nm InGaN light-emitting diodes", *J. Appl. Phys.*, **107**, 013103
35 (2010).
- 36 [23] W. Yang, S. Zhang, J. J. D. McKendry, J. Herrnsdorf, P. Tian, Z. Gong, Q. Ji,
37 I. M. Watson, E. Gu, M. D. Dawson, L. Feng, C. Wang, and X. Hu, "Size
38 dependent capacitance study on InGaN-based micro-light-emitting diodes", *J.*
39 *Appl. Phys.*, **116**, 044512 (2014).
- 40 [24] N. Otsuji, K. Fujiwara, and J. K. Sheu, "Electroluminescence efficiency of
41 blue InGaN / GaN quantum-well diodes with and without an n-InGaN
42 electron reservoir layer", *J. Appl. Phys.*, **100**, 113105 (2006).
- 43 [25] X. Ni, X. Li, J. Lee, S. Liu, V. Avrutin, U. Özgür, H. Morkoç, A. Matulionis, T.
44 Paskova, G. Mulholland, and K. R. Evans, "InGaN staircase electron injector
45 for reduction of electron overflow in InGaN light emitting diodes", *Appl. Phys.*
46 *Lett.*, **97**, 031110 (2010).
- 47 [26] W.-Y. Shiao, C.-F. Huang, T.-Y. Tang, J.-J. Huang, Y.-C. Lu, C.-Y. Chen, Y.-
48 S. Chen, and C. C. Yang, "X-ray diffraction study on an InGaN / GaN
49 quantum-well structure of prestrained growth", *J. Appl. Phys.*, **101**, 113503
50 (2007).

- 1 [27] D. S. Meyaard, G.-B. Lin, Q. Shan, J. Cho, E. Fred Schubert, H. Shim, M.-H.
2 Kim, and C. Sone, "Asymmetry of carrier transport leading to efficiency droop
3 in GaInN based light-emitting diodes", *Appl. Phys. Lett.*, **99**, 251115 (2011).
- 4 [28] X. Ni, Q. Fan, R. Shimada, U. m. Özgür, and H. Morkoç, "Reduction of
5 efficiency droop in InGaN light emitting diodes by coupled quantum wells",
6 *Appl. Phys. Lett.*, **93**, 171113 (2008).
- 7 [29] C. H. Wang, J. R. Chen, C. H. Chiu, H. C. Kuo, Y.-L. Li, T. C. Lu, and S. C.
8 Wang, "Temperature-dependent electroluminescence efficiency in blue
9 InGaN–GaN light-emitting diodes with different well widths", *IEEE Photon.*
10 *Technol. Lett.*, **22**, 236, (2010).
- 11 [30] M. F. Schubert and E. F. Schubert, "Effect of heterointerface polarization
12 charges and well width upon capture and dwell time for electrons and holes
13 above GaInN/GaN quantum wells", *Appl. Phys. Lett.*, **96**, 131102 (2010).
- 14 [31] C.-H. Chen, S.-J. Chang and Y.-K. SU, "High-Indium-Content InGaN/GaN
15 Multiple-Quantum-Well Light-Emitting Diodes", *Jap. J. Appl. Phys.*, **42**, 2281
16 (2003).
- 17 [32] M.-J. Lai, M.-J. Jeng, and L.-B. Chang, "High-Efficiency InGaN-Based
18 Yellow-Green Light-Emitting Diodes", *Jap. J. Appl. Phys.*, **49**, 021004 (2010).
- 19 [33] T. Takeuchi, C. Wetzel, S. Yamaguchi, H. Sakai, H. Amano, I. Akasaki, Y.
20 Kaneko, S. Nakagawa, Y. Yamaoka, and N. Yamada, "Determination of
21 piezoelectric fields in strained GaInN quantum wells using the quantum-
22 confined Stark effect", *Appl. Phys. Lett.*, **73**, 1691 (1998).
- 23 [34] J.-H. Ryou, P. D. Yoder, J. Liu, Z. Lochner, H. Kim, S. Choi, H. J. Kim, and R.
24 Dupuis, "Control of quantum-confined stark effect in InGaN-based
25 quantum wells," *IEEE J. Sel. Top. Quant. Electron.*, **15**, 1080 (2009).
- 26 [35] Y.-J. Lee, C.-H. Chiu, C. C. Ke , P. C. Lin, T.-C. Lu, H.-C. Kuo, and S.-C.
27 Wang, "Study of the excitation power dependent internal quantum efficiency
28 in InGaN/GaN LEDs grown on patterned sapphire substrate," *IEEE J. Sel. Top.*
29 *Quantum Electron.*, **15**, 1137 (2009).
- 30 [36] J.-H. Chen, Z.-C. Feng, H.-L. Tsai, J.-R. Yang, P. Li, C. Wetzel, T.
31 Detchprohm and J. Nelson, "Optical and structural properties of InGaN/GaN
32 multiple quantum well structure grown by metalorganic chemical vapor
33 deposition," *Thin Solid Films*, **498**, 123 (2006).
- 34 [37] Y. D. Qi, H. Liang, D. Wang, Z. D. Lu, W. Tang, and K. M. Lau,
35 "Comparison of blue and green InGaN/GaN multiple-quantum-well light-
36 emitting diodes grown by metalorganic vapor phase epitaxy," *Appl. Phys. Lett.*,
37 **86**, 101903 (2005).
- 38 [38] J.-Y. Zhang, L.-E. Cai, B.-P. Zhang, X.-L. Hu, F. Jiang, J.-Z. Yu, Q.-M. Wang,
39 "Efficient hole transport in asymmetric coupled InGaN multiple quantum
40 wells", *Appl. Phys. Lett.*, **95**, 161110 (2009).
- 41 [39] APSYS, Version 2008.06.01, Crosslight Software, Inc., Burnaby Canada,
42 1995–2005.
- 43 [40] Z.-M. Li, K. M. Dzurko, A. Delage, and S. P. McAlister, "A self-consistent
44 two-dimensional model of quantum-well semiconductor lasers: optimization
45 of a GRIN-SCH SQW laser structure", *IEEE J. Quant. Electron.*, **28**, 792
46 (1992).
- 47 [41] S. L. Chuang, and C. S. Chang, "A band-structure model of strained quantum-
48 well wurtzite semiconductors," *Semicond. Sci. Technol.*, **12**, 252 (1997).
- 49 [42] L. Liu, L. Wang, N. Liu, W. Yang, D. Li, W. Chen, Z. C. Feng, Y. C. L, I.
50 Ferguson, and X. Hu, "Investigation of the light emission properties and

1 carrier dynamics in dual-wavelength InGaN/GaN multiple-quantum well light
2 emitting diodes", *J. Appl. Phys.*, **112**, 083101 (2012).

3 [43] W. Yang, D. Li, N. Liu, Z. Chen, L. Wang, L. Liu, L. Li, C. Wan, W. Chen, X.
4 Hu, and W. Du, "Improvement of hole injection and electron overflow by a
5 tapered AlGaIn electron blocking layer in InGaIn-based blue laser diodes",
6 *Appl. Phys. Lett.*, **100**, 031105 (2012).

7 [44] M. Gladysiewicz, R. Kudrawiec, and M. S. Wartak, "Electronic Band Structure
8 and Material Gain of Dilute Nitride Quantum Wells Grown on InP Substrate",
9 *IEEE J. Quant. Electron.*, **51**, 7100212 (2015).

10 [45] B. Chen, W. Y. Jiang, and A. L. Holmes Jr., "Design of strain compensated
11 InGaAs/GaAsSb type-II quantum well structures for mid-infrared photodiodes",
12 *Opt. Quant. Electron.*, **44**, 103 (2012).

13 [46] B. Chen and A. L. Holmes Jr., "Optical gain modeling of InP based
14 InGaAs(N)/GaAsSb type-II quantum wells laser for mid-infrared emission",
15 *Opt. Quant. Electron.*, **45**, 127 (2013).

16 [47] Z. Yang, R. Li, Q. Wei, T. Yu, Y. Zhang, W. Chen, and X. Hu, "Analysis of
17 optical gain property in the InGaIn/GaN triangular shaped quantum well under
18 the piezoelectric field", *Appl. Phys. Lett.*, **94**, 061120 (2009).

19 [48] J.-R. Chen, C.-H. Lee, T.-S. Ko, Y.-A. Chang, T.-C. Lu, H.-C. Kuo, Y.-K.
20 Kuo, and S.-C. Wang, "Effects of built-in polarization and carrier overflow on
21 InGaIn quantum-well lasers with electronic blocking layers", *J. Lightwave
22 Technol.*, **26**, 329 (2008).

23 [49] F. Bernardini and V. Fiorentini, "Nonlinear macroscopic polarization in III-V
24 nitride alloys", *Phys. Rev. B*, **64**, 085207 (2001).

25 [50] J. P. Ibbetson, P. T. Fini, K. D. Ness, S. P. DenBaars, J. S. Speck, and U. K.
26 Mishra, "Polarization effects, surface states, and the source of electrons in
27 AlGaIn/GaN heterostructure field effect transistors", *Appl. Phys. Lett.*, **77**, 250
28 (2000).

29 [51] S. F. Chichibu, A. C. Abare, M. S. Minsky, S. Keller, S. B. Fleischer, J. E.
30 Bowers, E. Hu, U. K. Mishra, L. A. Coldren, S. P. DenBaars, and T. Sota,
31 "Effective band gap inhomogeneity and piezoelectric field in InGaIn/GaN
32 multi-quantum well structures ", *Appl. Phys. Lett.*, **73**, 2006 (1998).

33 [52] Y.-K. Kuo, M.-C. Tsai, S.-H. Yen, T.-C. Hsu, and Y.-J. Shen, "Enhancement
34 of Light Power for Blue InGaIn LEDs by Using Low-Indium-Content InGaIn
35 Barriers", *IEEE J. Sel. Top. Quant. Electron.*, **15**, 1115 (2009).

36 [53] I. Vurgaftman and J. R. Meyer, "Band parameters for nitrogen-containing
37 semiconductors ", *J. Appl. Phys.*, **94**, 3675 (2003).

38

The relation between k.p theory, self-consistent k.p theory and device simulation models:

1. Device simulation models:

The basic equations to describe the electrical behavior of device are the following:

a) Poisson's equation of electric potential V (field)

$$-\nabla \cdot \left(\frac{\epsilon}{q} \nabla V \right) = -n + p + N_D(1 - f_D) - N_A f_A + \sum_j N_{tj}(\delta_j - f_{tj}) + N_{it}$$

$$E = -\nabla V$$

n, p : electron and hole concentration, usually by injection;

N_D, N_A : donor and acceptor concentration;

N_{tj} : defect density for deep trap of j level;

N_{it} : interface charge density, for example, polarization charge.

b) Current continuity equations for electrons and holes

$$\nabla \cdot \left(\frac{j_n}{q} - R_{sp} - R_{st} - R_{auger} + G_{opt}(t) \right) = \frac{\partial n}{\partial t} + N_D \frac{\partial f_D}{\partial t}$$

$$\nabla \cdot \left(\frac{j_p}{q} + R_{sp} + R_{st} + R_{auger} - G_{opt}(t) \right) = -\frac{\partial p}{\partial t} + N_A \frac{\partial f_A}{\partial t}$$

The basic equations to describe optical behavior are:

c) Wave equation for light:

$$\nabla^2 W(x, y) + k_0^2 (\epsilon(x, y) - \beta^2) W(x, y) = 0$$

d) Photon rate equation

$$\frac{c}{\beta_1} \left[g_m - \frac{1}{2L} \ln\left(\frac{1}{r_m}\right) \right] S + c_m \int R_{sp} dv = 0$$

For light emitting devices, light output power (LOP) is very important. Basically, $LOP \propto R_{sp}$, where R_{sp} is the spontaneous recombination term. In a simple ABC model based on classical theory, $R_{sp} = Bn^2$, but it usually requires quantum mechanical

calculation of band structure in quantum wells (this is exactly what have been done in our simulation by k.p theory).

2. k.p theory:

k.p theory is a way to solve the Schrödinger equation in semiconductors to obtain band structure, wave function and recombination terms. It is a very old topic, while k.p theory for nitride was recently developed by S. L. Chuang. The k.p theory for nitride devices is slightly different from that for GaAs-based ones. One key issue is how to deal with polarization field, which was represented by the method by Bernardini, F. and V. Fiorentini (F. Bernardini and V. Fiorentini, “Nonlinear macroscopic polarization in III-V nitride alloys,” *Physics Review B*, Vol. 64, No. 8, pp. 085207 (2001)).

3. Self-consistent k.p theory

The self-consistent k.p theory just means a simultaneous solution of Schrödinger equation and Poisson equation. So our model is in nature a self-consistent k.p theory incorporated with more advanced models for nitride devices.

4. The methodology of using no polarization field as a reference in polar QWs

The methodology of using no polarization field as a reference in polar QWs has been accepted in many groups in the GaN community. Here give some researchers and references:

[1] Joachim Piprek, Robert Farrell, Steve DenBarrs, and Shuji Nakamura, “Effects of built-in polarization on InGaN-GaN vertical-cavity surface-emitting lasers”, *IEEE Photonics Technology Letters*, Vol. 18, No. 1, pp.7-9, 2006.

[2] Jun-Rong Chen, Chung-Hsien Lee, Tsung-Shine Ko, Yi-An Chang, Tien-Chang Lu, Hao-Chung Kuo, Yen-Kuang Kuo, and Shing-Chung Wang, “Effects of built-in polarization and carrier overflow on InGaN quantum-well lasers with electronic

blocking layers”, *Journal of Lightwave Technology*, Vol. 26, No. 3, pp.329-337, 2008.

[3] Ziwen Yang, Rui Li, Qiyuan Wei, Tao Yu, Yanzhao Zhang, Weihua Chen, and Xiaodong Hu, “Analysis of optical gain property in the InGaN/GaN triangular shaped quantum well under the piezoelectric field,” *Applied Physics Letters*, Vol. 94, No. 6, pp.061120, 2009.

5. Polarization charge, polarization field and screen effect

Polarization field includes piezoelectric polarization and also spontaneous polarization. Polarization field was equivalent to interface charges through Poisson equation:

$$\frac{\epsilon_0 \epsilon_{dc}}{q} \nabla \cdot \mathbf{E} = N_{it}$$

N_{it} stands for polarization charge at the interface. As there are defects, deep level traps, donor and acceptor (as shallow level traps) in the material. Even at zero bias where there is no current injection, the field is still screened. Therefore, the equation changes to:

$$\frac{\epsilon_0 \epsilon_{dc}}{q} \nabla \cdot \mathbf{E} = N_{it} - N_{defects}$$

According to experiment, the screen ratio is 20%-80%, and we set it at 50% in our work. Note that N_{it} and $N_{defects}$ generally do not move in the material and also do not change with current injection (so the screen ratio is relatively unchanged), that is

$$N_{it} = N_0 \delta(x - x_{it}), \forall j$$

When current density increases, free carriers such as electrons and holes increases, which can be calculated by current continuity equation:

$$\nabla \cdot \mathbf{j} - \frac{\partial n}{\partial t} - R_{sp} - R_{st} - R_{auger} + G_{opt}(t) = \frac{\partial n}{\partial t} + N_D \frac{\partial f_D}{\partial t}$$

In the steady state, electron or hole concentration is a function of space variable and current density $n(x, j)$. Because there exists the field, we have

$$n(x, j) \neq p(x, j), \forall x$$

Instead

$$\sum_x n(x, j) = \sum_x p(x, j), \forall j$$

Above is the charge neutrality condition in the device. So now the Poisson equation is

$$\frac{\epsilon_0 \epsilon_{dc}}{q} \nabla^2 \phi = \dots \quad \nabla_{defects} -n(x, j) + p(x, j),$$

We see how the screen ratio changes with current injection.

$$\begin{array}{l} \frac{\epsilon_0 \epsilon_{dc}}{q} \nabla^2 \phi \quad \dots \quad \xrightarrow{\text{screened by defects, deep/shallow level traps}} \\ \frac{\epsilon_0 \epsilon_{dc}}{q} \nabla^2 \phi \quad \dots \quad \nabla_{defects} \xrightarrow{\text{further screened by carrier/current injection}} \\ \frac{\epsilon_0 \epsilon_{dc}}{q} \nabla^2 \phi \quad \dots \quad \nabla_{defects} -n(x, j) + p(x, j) \end{array}$$

From both the current continuity equation and Poisson equation, generally we have

$$j \uparrow, n \uparrow, E \downarrow$$

This is the exactly way how we deal with this. Just as the Poisson equation introduced at the beginning:

$$\begin{aligned} -\nabla^2 \phi &= -n + p + N_D(1 - f_D) - N_A f_A + \sum_j N_{tj}(\delta_j - f_{tj}) + N_{it}, \\ E &= -\nabla V \end{aligned}$$

It should be emphasized that we make no hypothesis that the polarization charge N_{it} decreases with current injection.

From our previous paper (Z. Gong, et al., Semiconductor Science and Technology, Vol. 27, No. 1, pp. 015003 (2011)), we get a formula between E and j as a parabolic fit. The fit is empirical, and may be valid for only certain devices. A standard and self-consistent way is to solve the Poisson equation and current continuity equation.