Effect of Quantum Barrier Thickness in the Multiple-Quantum-Well Active Region of GaInN/GaN Light-Emitting Diodes

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DOI: 10.1109/JPHOT.2013.2276758
1943-0655 © 2013 IEEE

Manuscript received July 12, 2013; revised July 29, 2013; accepted July 30, 2013. Date of publication August 7, 2013; date of current version August 16, 2013. This work was supported by Samsung Electronics Company, by the Basic Science Research Program through the National Research Foundation (NRF) (2010-0006646) and by Applied Materials–Varian Semiconductor Equipment. The work of J. Cho was supported by the Basic Research Laboratory Program (2011-0027956) and Priority Research Centers Program (2009-0094031) through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology. Corresponding authors: J. Cho and J. K. Kim (e-mail: cho.jaehee@gmail.com; kimjk@postech.ac.kr).

Abstract: The dependence of the polarization-induced electric field in GaInN/GaN multiple-quantum-well light-emitting diodes (LEDs) on the GaN quantum barrier (QB) thickness is investigated. Electrostatic arguments and simulations predict that a thin QB thickness reduces the electric field in the quantum wells (QWs) and also improves the LED efficiency. We experimentally demonstrate that the QW electric field decreases with decreasing QB thickness. The lower electric field results in a better overlap of electron and hole wave functions and better carrier confinement in the QWs. A reduced efficiency droop and enhanced internal quantum efficiency is demonstrated for GaInN/GaN LEDs when the QB thickness is reduced from 24.5 to 9.1 nm.

Index Terms: Light emitting diode, gallium nitride, efficiency droop.

1. Introduction

III-nitride semiconductors have a strong polarization along the c-direction due to their wurtzite crystal structure, and the polarization is determined by the chemical composition of the semiconductor as well as strain distorting the crystal lattice [1]. Therefore, polarization-induced charges exist at hetero-interfaces of III-nitride semiconductors grown along the *c* axis; for example, polarization charges exist at the GaInN/GaN QW/QB interface and at the GaN/AlGaN spacer-layer/electron-blocking-layer (EBL) interface in multiple quantum well (MQW) light-emitting diodes (LEDs). The strong electric field in GaInN QWs is highly undesirable due to the following reasons: (1) a low internal quantum efficiency (IQE) is caused by the quantum-confined Stark effect (QCSE); (2) severe electron leakage is caused by the reduced dwell time of electrons above GaInN QWs and inefficient carrier confinement [2]. Moreover, the polarization-induced electric field is regarded as an important cause of the well-known light-output-loss mechanism at high currents, known as the efficiency droop [2]–[4].

Many efforts have been made to reduce or even eliminate the polarization-induced electric field in GaInN QWs, for example, by matching the polarization of individual QB and QW layers of the MQW active region by utilizing ternary GaInN or quaternary AlGaInN QBs [3]–[5], or by growing LED epitaxial layers on semi-polar or non-polar substrates [6]–[9], or by the band structure engineering of QW region [10]–[14]. It is notable that a blue-shift of the photoluminescence and electroluminescence from $\mathrm{Ga_xIn_{1-x}N}$ QWs was reported for decreasing thickness of the GaN or AlGaN QBs [15]–[19], indicating that the electric-field in the QWs as well as the performance of III-nitride LEDs is sensitive to the QB thickness. This motivates our present investigation of the effect of GaN QB thickness on the polarization-induced electric field in GaInN QWs and its correlation with the optical performance of LEDs. In this paper, we use simulations as well as electrostatic arguments to show how the control of the QB thickness allows us to reduce the electric field in the GaInN QWs. In addition, we present experimental results showing the influence of the QB thickness on the IQE, on the emission wavelength shift with injection current, and on the efficiency droop.

2. Theoretical Analysis

In order to understand the effect of the QB thickness on the polarization-induced electric field in the QWs, let us consider an MQW structure without a built-in pn-junction potential and without an externally applied voltage, so that the polarization-induced sheet charges at the QB/QW hetero-interfaces are the only source of electric field. In such an MQW structure, the net charge, and hence the total potential drop across one MQW period, is zero, that is

$$d_{\mathrm{QW}} E_{\mathrm{QW}} + d_{\mathrm{QB}} E_{\mathrm{QB}} = 0 \tag{1}$$

where E_{QW} and E_{QB} are the electric fields in the QW and QB having a thickness of d_{QW} and d_{QB}, respectively. Moreover, the divergence of electric displacement field (D) is equal to the charge density ($\bigtriangledown \cdot D = \rho$). Therefore, the boundary condition for the electric displacement field at the QW/QB hetero-interface is,

$$-\epsilon_{\mathrm{QW}} E_{\mathrm{QW}} + \epsilon_{\mathrm{QB}} E_{\mathrm{QB}} = -\sigma \approx \epsilon_{\mathrm{QW}} (E_{\mathrm{QW}} - E_{\mathrm{QB}}) \tag{2}$$

where σ is the interface charge density at the QW/QB interface, and ϵ_{QW} and ϵ_{QB} are the dielectric permittivity of the $\mathrm{Ga_{0.85}In_{0.15}N}$ QW and GaN QB material, respectively, and we assume that $\epsilon_{\mathrm{QW}} = 9.7 \times \epsilon_0 \approx \epsilon_{\mathrm{QB}} = 8.9 \times \epsilon_0$. Solving Eqns. (1) and (2) for the electric fields in the QB and the QW, we obtain

$$E_{\mathrm{QB}} \approx -\frac{\sigma}{\epsilon_{\mathrm{QW}}} \frac{1}{1 + (d_{\mathrm{QB}} + d_{\mathrm{QW}})} = -E_0 \frac{1}{1 + (d_{\mathrm{QB}}/d_{\mathrm{QW}})} \tag{3}$$

$$E_{\mathrm{QW}} \approx -\frac{\sigma}{\epsilon_{\mathrm{QW}}} \frac{1}{1 + (d_{\mathrm{QW}} + d_{\mathrm{QB}})} = +E_0 \frac{1}{1 + (d_{\mathrm{QW}}/d_{\mathrm{QB}})} \tag{4}$$

where we define $E_0 = \sigma/\epsilon_{\mathrm{QW}}$. For example, the polarization charge density σ is calculated to $2.42 \times 10^{-2}\ \mathrm{C/m^2}$ at the $\mathrm{Ga_{0.85}In_{0.15}N}$/GaN interface and $E_0 \approx 2.81$ MV/cm [20]. Equation (4) shows that the polarization field in the GaInN QWs of GaInN/GaN MQW structures can be reduced by decreasing the QB/QW thickness ratio.

Energy band diagrams and the IQE of GaInN/GaN MQW structures with various QB thicknesses are simulated by Advanced Physical Models of Semiconductor Devices (APSYS) software. The simulated LED has an epitaxial structure of a 3-μm-thick n-type GaN layer (donor concentration $= 3.7 \times 10^{18}\ \mathrm{cm^{-3}}$), a MQW active region, a 15-nm-thick last-grown barrier, a 30-nm-thick p-$\mathrm{Al_{0.19}Ga_{0.81}N}$ electron-blocking layer (acceptor concentration $= 1.0 \times 10^{18}\ \mathrm{cm^{-3}}$), and a 100-nm-thick p-type GaN layer (acceptor concentration $= 1.0 \times 10^{19}\ \mathrm{cm^{-3}}$). We use three MQW active region designs consisting of three 3-nm-thick $\mathrm{Ga_{0.85}In_{0.15}N}$ QWs and two (i) 4-nm-, (ii) 8-nm-, and (iii) 16-nm-thick GaN QBs located between the QWs. These three structures are used to study

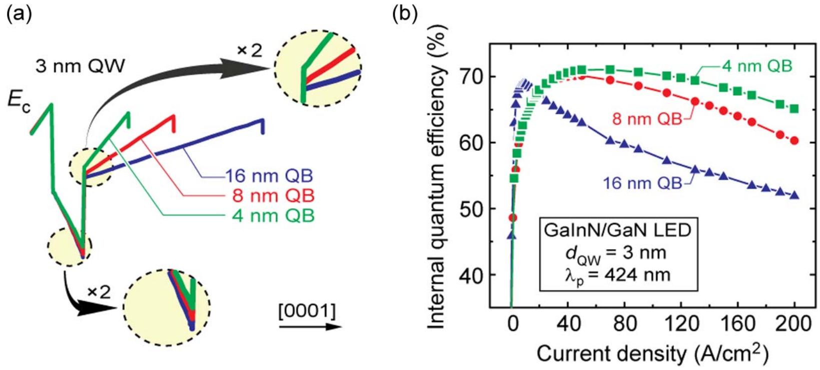

Fig. 1. (a) Calculated conduction-band energy of a GaInN/GaN MQW structure with a 3 nm thick QW and with 4 nm, 8 nm, and 16 nm thick QBs. With decreasing QB thickness, the internal electric field in the QW becomes smaller (smaller slope of E_c in the magnified lower circle), causing a smaller potential difference across the QW (the upper circle). (b) Simulated IQE-versus-current-density curves of GaInN/GaN MQW LEDs having three QWs (3 nm thick) and 4 nm, 8 nm, and 16 nm thick QBs.

the effect of QB thickness. We use the AlGaN, GaN, and GaInN material parameters published by Piprek [21]. Fig. 1(a) shows the conduction band edge, E_c, of a $Ga_{0.85}In_{0.15}N$/GaN MQW structure having 4-nm-, 8-nm-, and 16-nm-thick QBs. In the figure, we align the left-hand interface between the GaN QB layer and the GaInN QW to investigate the change in slope of E_c. The slope of E_c reveals the strength of the electric field in the QW and QB. With decreasing QB thickness, the electric field in the QW decreases, while that in the QB increases. The magnifying lower circle shown in Fig. 1(a) elucidates that the thinner QB has the smaller slope of E_c in the QW, which means the smaller electric field in the QW, and is consistent with Eq. (4). Simultaneously, the slope of E_c in the QB becomes steeper, i.e., the electric field in the QB becomes larger, when decreasing the QB thickness, as shown in the magnifying upper circle of Fig. 1(a). Fig. 1(b) shows the simulated IQE-versus-current-density curves of LEDs with a 3-period GaInN/GaN MQW active region consisting of 3-nm-thick QWs with 4-nm-, 8-nm-, and 16-nm-thick QBs. As the QB thickness decreases, the overall IQE increases and the efficiency droop becomes less severe, which we attribute to the smaller electric field in the QWs. The smaller electric field in the QWs contributes to a higher IQE due to an enhanced overlap of electron and hole wave functions. In addition, the smaller QW field also enables a lower efficiency droop due to a longer dwell time of carriers over the QWs [2]. In Fig. 1(a), one can notice a smaller potential difference across QW for a thinner barrier; less kinetic energy is gained by carriers when traversing a QW. For a given QW thickness, less kinetic energy implies a higher probability of an electron being captured by the QW, i.e., less electron leakage. As a result, fewer carriers leak out and more carriers stay in the active region and contribute to radiative recombination; therefore, the droop-onset current can be raised and higher peak IQE is expected [3].

3. Experimental Details

For experimental verification of the above-detailed electrostatic arguments and of the simulation results, a series of GaInN/GaN MQW LEDs with three different QB thicknesses was grown by metal-organic vapor phase epitaxy (MOVPE) on *c*-plane sapphire substrates. All epitaxial layers consist of 2 μm undoped GaN, 2 μm Si-doped GaN, an MQW structure with three periods of $Ga_{0.85}In_{0.15}N$/GaN QWs and QBs, a 10 nm undoped GaN spacer, a 10 nm Mg-doped $Al_{0.1}Ga_{0.9}N$ EBL, and a 100 nm Mg-doped p-type GaN layer. The thickness of the QBs was the only difference between the three samples. The QW growth time was fixed for all the samples while QB growth time was 2, 6, and 16 minutes, respectively.

Here the samples are labeled, for the long, intermediate, and short QB growth time, as QB1, QB2, and QB3 sample, respectively. After the epitaxial growth, all three samples were fabricated in the same processing run. First, the mesa structure was etched by inductively-coupled plasma

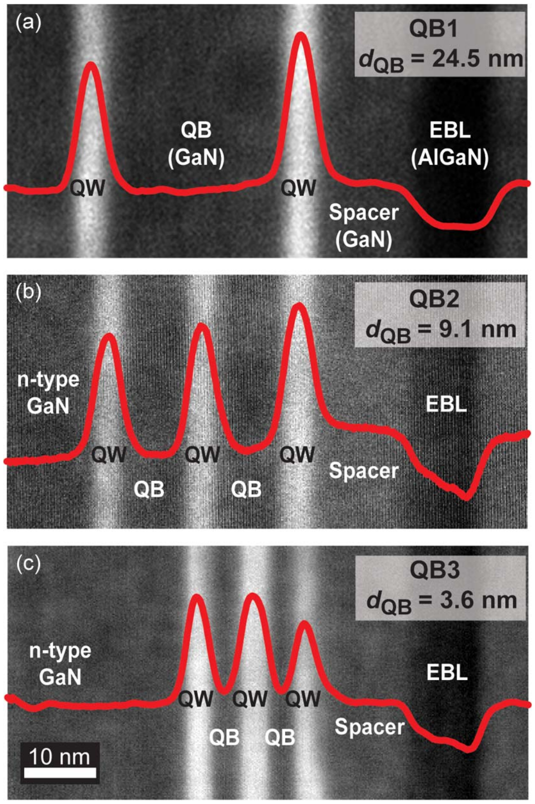

Fig. 2. HAADF-STEM cross-sectional images of (a) QB1, (b) QB2, and (c) QB3 samples with averaged HAADF intensity profiles (red lines). The QW thickness is measured to be 4.2 ± 0.2 nm, and the QB thicknesses are estimated, by subtracting the GaInN QW thickness from the QW + QB thickness, to be 24.5 nm, 9.1 nm, and 3.6 nm for QB1, QB2, and QB3, respectively.

reactive-ion etching using BCl_3/Cl_2 gas chemistry. Then, a Ti/Al (30/250 nm) n-type ohmic contact was deposited by electron-beam evaporation and subsequently annealed at 650 °C for 1 minute in a N_2 ambient. A NiZn/Ag (5/200 nm) p-type ohmic contact was deposited by electron-beam evaporation, followed by annealing in air at 500 °C for 1 minute. The thicknesses of the QBs and QWs for each of the three LED samples were measured by using high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM).

4. Results

Fig. 2 shows the HAADF STEM images of the QB1, QB2, and QB3 samples. The HAADF intensity is approximately proportional to the square of atomic number, so the brighter regions represent the GaInN QWs while the darker regions represent the GaN QBs. The QB thicknesses were measured, by subtracting the QW thickness (4.2 ± 0.2 nm) from the QW + QB thickness which is the period between HAADF intensity peaks; using this procedure, we obtained a QB thickness of 24.5, 9.1, and 3.6 nm for the QB1, QB2, and QB3 sample, respectively.

To estimate the electric field in the QWs, current-density-dependent emission spectra were measured using a spectrometer. Fig. 3(a) shows the peak wavelength at 10 and 100 A/cm^2 as a function of the QB thickness. At a low current density such as 10 A/cm^2, carriers in the active region are strongly influenced by the internal electric field in the QWs. Thicker QBs generally result in a larger internal electric field in the QWs. This causes a smaller optical transition energy due to a large QCSE, so that the peak wavelength becomes longer with increasing QB thickness. However, at the high current density of 100 A/cm^2, the QW electric field is screened, and therefore, the peak wavelength is independent of QB thicknesses, consistent with Fig. 3(a). Considering the lack of

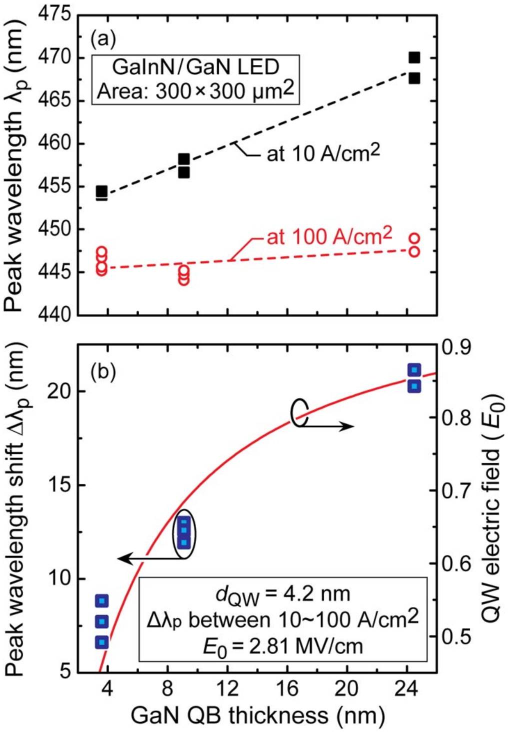

Fig. 3. (a) Peak emission wavelengths of GaInN/GaN LED at 10 A/cm^2 and 100 A/cm^2 as a function of the GaN QB thickness in the MQW active region. (b) Measured peak wavelength shift incurred when increasing the current density from 10 to 100 A/cm^2 for samples with different QB thickness. The solid curve shows the electric field calculated by Eq. (4).

field-dependence of the peak wavelength at high currents as a reference, the difference between the strongly-field-dependent peak wavelength at low currents and the field-independent peak wavelength at high currents allows one to estimate the electric field in the QWs. Fig. 3(b) shows the shift of the peak emission wavelength, $\Delta\lambda_p$, as a function of the QB thickness when increasing the current density from 10 to 100 A/cm^2. The larger peak-wavelength shift for thick-QB samples indicates that the energy band bending and the electric field in the QWs become larger with increasing QB thickness. The solid line in Fig. 3(b) represents the electric field calculated from Eq. (4), and the tendency displayed in the figure is consistent with the above-articulated argument on the peak-wavelength shift.

Fig. 4(a) shows that the external quantum efficiency (EQE) for the three LED samples as a function of injection current. Comparing sample QB2 with sample QB1 shows that, as the QB becomes thinner, the efficiency droop at 200 mA strongly decreases from 18.1% to 9.4%. In addition, for a thinner QB, a delay in the droop onset is expected because a smaller QW field can reduce the carrier leakage and increase carrier dwell time. Indeed, the droop-onset current (peak-efficiency current) is raised from 35.2 mA to 48.2 mA. Recently, carrier leakage was proposed as the main reason for the efficiency droop [3]. A lower carrier leakage allows for a higher peak IQE. As a result, the peak-efficiency is increased by 2.2% for sample QB2 with thinner QB. QB3 LED has an even lower efficiency droop (0.8%) and a much higher droop-onset current (158 mA). However, the peak efficiency of the QB3 LED is somewhat lower than that of the QB1 and QB2 LEDs, thereby deviating from the theoretical expectation. For the QB3 LED with the thinnest GaN QB (3.6 nm), we believe that we reach the capability limit of our MOVPE system. Presumably, (i) a delicate interface-quality control will be required for the extremely thin QB sample to fulfill the theoretical expectation; (ii) such a thin QB could give a probability for intra-band tunneling between QWs which is not included in our calculation and simulation.

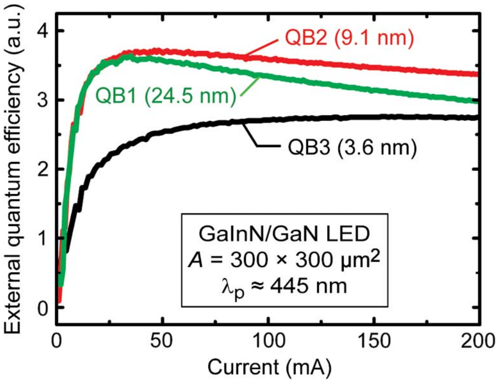

Fig. 4. Measured external quantum efficiency as a function of forward current for GaInN/GaN MQW LED samples with three different QB thicknesses (24.5 nm, 9.1 nm, and 3.6 nm).

5. Conclusion

In summary, we investigate the effect of GaN QB thickness on the electric field in GaInN QWs as well as on the efficiency of GaInN/GaN MQW LEDs. Based on electrostatic arguments, we develop the analytic relation between polarization-induced electric field and the QW and QB thicknesses. This relation shows that thinner QBs result in a smaller electric field in the QWs of an MQW structure. Simulations support the dependence of the QW electric field, i.e., thinner QBs result in a smaller electric field in the QWs. The smaller electric field in the QWs leads to a better efficiency performance and better carrier confinement due to a smaller QCSE. Moreover, a longer carrier dwell time over the QW caused by the smaller QW field reduces carrier leakage and the efficiency droop. Both simulations and experiments demonstrate that such positive effects can be attained for LED samples with a thin QB. In our experiments, we grow and fabricate three types of LEDs with fixed QW thickness (4.2 nm) and three different QB thicknesses which were determined by HAADF-STEM to be 24.5, 9.1, and 3.6 nm for sample QB1, QB2, and QB3, respectively. The LED with the thinner QB has smaller efficiency droop and larger onset current of the efficiency droop. The efficiency droop at 200 mA is 18.1%, 9.4%, and 0.8% for QB1, QB2, and QB3 LED, respectively. In addition, the onset current of the droop is 35.2 mA, 48.2 mA, and 158 mA for QB1, QB2, and QB3 LED, respectively. The results show that a thin QB thickness provides an efficient and practical way for enhancing efficiency performance of GaInN/GaN LEDs.

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