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Hsin-Hung Yao, Yi Lu, Kuang-Hui Li, Feras Al-Qatari, Che-Hao Liao, Xiaohang Li, "Polarization matched c-plane III-nitride quantum wells structure," Proc. SPIE 10940, Light-Emitting Devices, Materials, and Applications, 109400K (1 March 2019); doi: 10.1117/12.2509873

SPIE.

Event: SPIE OPTO, 2019, San Francisco, California, United States

Polarization matched *c*-plane III-nitride quantum wells structure

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ABSTRACT

Polarization-matched quantum wells (QWs) can lead to maximized electron-hole wave functions overlap and low efficiency droop at high current density. By using the modern theory of polarization with hexagonal reference, *c*-plane InAlN/InGaN QWs were explored and designed for polarization matching. The simulation results show that, even on *c*-plane, polarization-matched structures can be achieved by adjusting strain and material composition. The In composition of larger than 35% of InAlN was required to match the total polarization of InGaN at any given composition. Considering the bandgap's bowing factors of III-nitride ternary alloys, In_{0-0.1}Ga_{1.0-0.9}N as quantum barrier (QB) provided enough potential barriers for In_{0.35-0.45}Al_{0.65-0.55}N to form a multiple QW (MQW) structure. The results indicated that improper resistance of MQW and the existing fixed charge between the interfaces of p-type region/MQW and n-type region/MQW could result in nonuniform carrier distributions and current leakage, respectively. Furthermore, we found that In_{0.41}Al_{0.59}N/In_{0.1}Ga_{0.9}N polarization-matched MQW had proper resistance; however, such structure produced a huge polarization fixed-charge between the junction interface. By studying the strain level of InAlN QW and GaN QB, which can be grown on AlN/GaN superlattice templates, the In_{0.33}Al_{0.67}N/GaN polarization-matched MQW structure has been specifically designed with small resistance and without inducing improper polarization fixed charge. By optimizing the number and thickness of QWs, the 425nm LED has relative IQE of 56% and efficiency droop of only 7% at high current density of 333 A/cm². This study provides guidance for development of In-rich InAlN materials.

Introduction

Gallium nitride materials have received much attention for decades and have been achieved great success in the field of solid-state lightingⁱ. In these decades of development, the high external quantum efficiency and high wall plug efficiency of GaN blue light emitting diodes (LEDs) have been developed. A large part of these successful developments is due to the advancement of epitaxy technology of nitride-based materialⁱⁱ. In recent years, the epitaxial technology of nitride-based material has been transferred from mature GaN and InGaN materials to the ternary alloy of Al-rich AlGaN

and InAlN materials^{iii,iv,v} and quaternary alloy of InAlGaN material to widen its application field and improved device performance.

In addition to epitaxy technology of nitride-based material, the theory of polarized electric field of nitride-material has been deeply studied and applied to improve the performance of devices. The polarization-induced surface charges at the heterointerfaces between the nitride materials modify the energy band and induce the quantum-confined Stark effect (QCSE) and increase the carrier leakage of multi-quantum well (MQW) of nitride-based LEDs^{vi}. About these studies, polarization-matched QWs have been receiving attention because it can maximize electron-hole wave functions overlap^{vii}. This is also the reasons of quaternary aluminum indium gallium-nitride (AlInGaN) has attracted much attention^{viii,ix,x}. Since strain-free heterostructures can be achieved by varying the composition of In, Al, and Ga from which nitrides. From YK, Kuo's report^{xi}, the In content of InGaN is 18% for blue LED, the Al and In contents of AlInGaN for polarization-matched design are both about 35% with the best performance characteristic. The AlInGaN materials with such content are difficult to develop the proper growth condition^{xii}. Especially as QBs layer, it is needed thicker thickness compared with QWs layer. InAlN compound with 18% In composition have attracted the attention of many researchers due to the lattice matching to GaN. This has led to two interest areas, Distribution Bragg reflectors (DBRs) and HEMTs. Actually, ternary InAlN materials can cover same range of bandgap and polarization field as AlInGaN materials, also very promising as a polarization-matched MQW structure. Recently, using InAlN as QW layers with the strong RT luminescence has been observed^{xiii}.

Recently, David Vanderbilt's group has proposed a modern polarization electric field model that conforms to the growth of the nitride material on *c*-plane^{xiv}. They used the hexagonal reference structure instead of the zincblende reference structure that has been used to calculate the polarization field constant on the C-axis of the nitride-based material. Compared with these values of polarization constant of III-nitrides calculated by zinc blende (ZB) reference structure conventionally used, a rigorously correct value of polarization constant of III-nitrides has been provided by hexagonal reference structure. With our past calculation of the value of the III-nitride polarization constant^{xv}, a significant correction

appears in the calculation of spontaneous polarization (SP) and the SP direction is the same as (0001). In this paper, we used h-reference polarization model to calculate the total polarization of InGaN and InAlN materials, and based on these results, InAlN/InGaN polarization match MQW structures have been designed. In this study, InAlN was used as the active layer, and the LED performance was studied and investigated. Compared with the conventional GaN/InGaN MQW light-emitting layer, the InAlN/InGaN MQW LED devices were demonstrated to be able to further increase the efficiency, reduce the efficiency droop under high current density drive.

STRUCTURES AND METHOD

Structures investigated in this paper were all designed on c-plane template and used a commercial technology computer-aided design (TCAD) software, Advanced Physical Models of Semiconductor Devices (APSYS) developed by Crosslight Inc., to simulate the LEDs' optical and electrical properties. The simulated LED structures designed with a chip size of $300 \times 300 \mu\text{m}^2$ and carrier injected way with a vertical path. Ideal ohmic contacts are assumed to cover the full top and bottom p-contact and n-contact layers, respectively. Utilizing such a design structure to obtain a uniform current distribution to eliminate the issue of current crowding. The nitride-based LED structures were grown on an n-GaN template and the n-side structure of the LEDs consists of a 3- μm -thick n-type GaN layer (3- μm , $[\text{Si}] = 5 \times 10^{18} \text{ cm}^{-3}$) as n-contact layer, and then a 500nm n-GaN (500nm, $[\text{Si}] = 3 \times 10^{17} \text{ cm}^{-3}$) as electron-injection layer. The p-side structure of the LEDs consists of a p-Al_{0.2}Ga_{0.8}N (20 nm, $[\text{Mg}] = 3 \times 10^{19} \text{ cm}^{-3}$) EBL layer, a p-GaN (150 nm, $[\text{Mg}] = 3 \times 10^{19} \text{ cm}^{-3}$) hole-injection layer, and finally a p⁺-GaN (50 nm, $[\text{Mg}] = 1 \times 10^{20} \text{ cm}^{-3}$) as contact layer. The active regions of the LEDs are consisting of six-period InAlN QWs (3 nm each) which divided by seven InGaN QBs (12 nm each) directly on the n-GaN layer. For modeling, Shockley-Read-Hall (SRH), Auger recombination, and radiative recombination coefficients were set to be $5 \times 10^7 \text{ 1/s ns}$, $6.0 \times 10^{-31} \text{ cm}^6/\text{s}$, and $1.0 \times 10^{-11} \text{ cm}^3/\text{s}$, respectively^{xvi}. In this simulation, the influence of crystalline quality is not taken into consideration, therefore the SRH coefficients and Auger recombination coefficients are assumed to be the same for all the structures under this report. The band offset ratio is set to 0.7/0.3^{xvii,xviii}, respectively. The charge density

screened by the injected charge carriers is determined self-consistently at different injection levels. Other material parameters used in the simulation can be referred to Ref. 19^{xix}.

Results and discussion

The total polarization (P_{total}) calculated results of InAlN and InGaN layers grown on a fully relaxed GaN template are shown in Fig. 1. Because of using H-reference structure, the direction of the polarization field in the material is (0001). In Fig. 1, the In composition (In%) of InAlN materials less than 18% are subjected to tensile strain. Other materials are subjected to compress strain which increases with In% increasing. However, the SP is decreased as In% increasing in InGaN and InAlN materials¹¹, it means that for P_{total} , the impact from strain effect is faster than the change of SP. As seen in Fig. 1, The InAlN of larger than 35% of In composition was required to match the P_{total} of InGaN at any given composition. Considering the critical thickness of the material due to lattice mismatch, the In composition range of InGaN is 0%~10%, and for InAlN is 35%~41%.

Figure 1 Calculated total polarization of AlInN and InGaN as a function of In composition on GaN template, dot line indicates the smallest P_{total} of polarization-matched region

On the fully relaxed GaN template, three polarization-matched MQW structures have been designed. By using GaN, $\text{In}_{0.05}\text{Ga}_{0.95}\text{N}$ and $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ as the QB layers and calculating the P_{total} (shown in Fig. 2), the polarization-matched MQW

structures on a fully relaxed GaN template have been obtained as $(\text{In}_{0.35}\text{Al}_{0.65}\text{N}/\text{GaN})$, $(\text{In}_{0.39}\text{Al}_{0.61}\text{N}/\text{In}_{0.05}\text{Ga}_{0.95}\text{N})$, and $(\text{In}_{0.41}\text{Al}_{0.59}\text{N}/\text{In}_{0.1}\text{Ga}_{0.9}\text{N})$. The wavelengths of these three MQW structures are 445nm, 486nm, and 515nm, respectively.

Figure 2 Polarization-matched InAlN/InGaN MQW designed. In composition of InGaN is 0%, 5%, and 10%, corresponding In composition of InAlN is 35%, 39%, and 41%,

The band diagram indicates that as increasing In% of QB structures, the barrier potential of polarization-matched MQW is decreasing while the resistance of MQW structures should be decreased. However, the discontinuity of band structure at the junction interfaces of LEDs gets larger as increasing In% of barrier materials, which also increases the polarization fixed charge between the interface. By chosen the $(\text{In}_{0.41}\text{Al}_{0.59}\text{N}/\text{In}_{0.1}\text{Ga}_{0.9}\text{N})$ MQW to form a LED structure, and the detail LED structures are plotted in Fig. 3. From the picture, the discontinuity of band structure at the junction interfaces of LEDs gets larger as increasing In% of barrier materials, which also increases the polarization fixed charge between the interface. Fig. 4(a) are the band diagram calculated results of Sample A at 300mA, respectively. The applied voltage on MQW structure and MQW resistance is (0.34V, 1.16Ω) for Sample A. However, the MQW resistance of Sample A is not small enough, and too large potential barrier is not conducive to the carriers' uniform distribution.

Figure 3 LED structure with $\text{In}_{0.41}\text{Al}_{0.59}\text{N}/\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ polarization-matched MQW structures.

So, the carrier's accumulating is happened and accumulating at the last QW. The increase of the QBs' In% also increases the polarization induced fixed-charges between the p-i-n interfaces. This intense charge will pull down the energy band and gather carrier at the interfaces of p-type region/MQW and n-type region/MQW resulted in leakage current generation. As seen in Fig. 4(b) and (c), the current leakage gets severe as increasing In% InGa_{0.9}N QBs.

Figure 4 (a) Band diagrams of Sample A, (b) Electron [e^-], and (c) Hole [h^+] concentration at 300mA

Another part of study, the P_{total} of materials can be modified by the strain level, it means that the P_{total} of InAlN/GaN MQW structure is different on various template structures. Therefore, the In% of InAlN QWs which polarization is matched to

GaN QBs could be modified by designed bottom template structure. Two templates, $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ have been chosen, and these two templates can be achieved by inserting InGaN/GaN SLs and AlN/GaN SLs between n-GaN and MQW structures, respectively. Although the SLs structure will be in the path of the injection current, it can be adjusted the thickness and doping level of each layer to minimize the effect on the LED performance. According to the calculation results of P_{total} shown in Fig. 5, applying tensile strain, the case of $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ template, the P_{total} of GaN QBs are reduced. And applying compress strain to GaN ($\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ template) increases the P_{total} . To get the low potential barrier MQW structure needs to decrease the In% of InAlN QW layers, the polarization-matched $\text{In}_{0.33}\text{Al}_{0.67}\text{N}$ /GaN MQW, Sample B, has been designed on an $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ template. Fig. 6 is the detail LED structure of Sample B, and the MQW ΔE_g of Sample F is 0.57eV similar to Sample A, and the emitted wavelength is 417nm.

Figure 5 Polarization-matched InAlN/GaN MQW designed on $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ template, GaN template, and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ template, and corresponding In composition in InAlN well is 38%, 35%, and 33%, respectively.

The simulation result of Sample B at 300mA shown in Fig. 7. From the band diagram (Fig. 7(a)), the applied voltage on the MQW structure and resistance of MQW structure is (0.34V, 1.13 Ω). The Sample B's MQW resistance is very similar with of Sample A, it means that the resistance of polarization-matched MQW structures is determined by barrier potential and less affected by polarization fixed charges between the p-i-n interfaces. Since the MQW resistance is similar, the carrier distribution of Sample B (Fig. 9(b)) is similar to that of Sample A, except that there is no leakage current induced

Figure 6 LED structure of Sample F with $\text{In}_{0.33}\text{Al}_{0.67}\text{N}/\text{GaN}$ polarization-matched MQW structures on $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ template.

by the fixed charge.

Figure 7 Calculated (a) Band diagrams (b) Electron $[n^-]$ and hole $[p^+]$ concentration of Sample B at 300mA,

As the electrons and holes are gathered in the last QW, it causes a droop effect due to the increasing of Auger recombination rate at high current. Comparing the LEDs' performances of Sample A ($\eta_{\text{peak}} = 57.8\%$, droop = 25.1%), and Sample B ($\eta_{\text{peak}} = 59.6\%$, droop = 20.1%), shown in Fig. 8, to consider the issue of fixed charges between the p-i-n interfaces can intensely improve LED performance and reduce droop effect.

Due to the recognition that the flexibility to design the correct resistance for the polarization-matched MQW is limited. The next part is to optimize the performance by pair number and thickness of QWs to the polarization-matched

MQW which with improper resistance. Since we already know that the unperfect performance of Sample F is because the resistance of MQW is not low enough, the pair number of MQW should be reduced. Fig. 9 shows the influence of the

Figure 8 IQEs and I-V curves of Samples A, and B at 300mA.

QWs number on the LED performance of Sample B. Fig. 0(a) shows the IQE as a function of injection current, and Fig 9(b) is the η_{peak} and $\eta_{300\text{mA}}$ as a function of the QWs number. The η_{peak} and the rate at which performance rises at low currents increases as the pair number decreased. However, lead to the droop become large with decreasing the QW pairs. As the results, 4-pair QWs structures are the optimal design for MQW of Sample B.

Figure 9 Calculated (a) IQE curve of 2-pair, 4-pair, and 6-pair $\text{In}_{0.33}\text{Al}_{0.67}\text{N}/\text{GaN}$ MQW structure (b) IQE at 300mA and maximum IQE with varied pairs of MQW.

Since polarization-matched $\text{In}_{0.33}\text{Al}_{0.67}\text{N}/\text{GaN}$ MQW does not have the QCSE effect, $[e^-]$ and $[h^+]$ can be adjusted by QW thickness and should not decrease the LED performance. Fig. 9(b) is the QW width effect on the LED performance of Sample F with 4-pair MQW structure. As expected, the efficiency droop is markedly improved with thick QW. In addition,

the value of η_{peak} slightly increases as the QW thickness increasing. It is because of $\text{In}_{0.33}\text{Al}_{0.67}\text{N}/\text{GaN}$ QW designed as a small potential barrier and decreases the carrier confined ability. However, as the QW thickness increasing, the carrier confined ability of QW structure will increase. The insert figure of Fig 10 is the ratio of actual QW width to the effective QW width under different well widths and compared it with the value of η_{peak} . The effective well width is calculated from the reference website (<http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/pfbox.html>). Generally, the nitride-based MQW structure because has a built-in electric field in QW structure, due to the QCSE effect, the IQE performance will decrease as the QW thickness increases. However, for a polarization-matched MQW structure, while designing a suitable MQW resistance to reduce the barrier potential, the thickness of the QW must also be considered to optimize the carrier confinement. From the above discussion, the performance of LEDs with polarization-matched $\text{In}_{0.33}\text{Al}_{0.67}\text{N} / \text{GaN}$ MQW structures can be more suitable for high current operation by optimizing the number and width of MQW structures. By considering the rate at which performance rises at low currents and the droop effect at high currents, for the case of 4-pair $\text{In}_{0.33}\text{Al}_{0.67}\text{N}/\text{GaN}$ QWs with 5nm on $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ template, which emitted wavelength is 425nm, the η_{peak} and droop is 62.6% and 16.0%, respectively. This design can be applied to the widest operating current condition.

Figure 10 Calculated IQE curve of different QW thickness (3nm, 5nm, and 7nm). The insert figure is the effective thickness ratio and maximal IQE under varied thickness of QW.

Conclusion

Nitride-based LEDs with Polarization-matched InAlN/InGaN MQW have been studied by using the modern theory of polarization with hexagonal reference. The characteristics of InAlN/InGaN polarization-matched MQW LEDs with various QBs and QWs were investigated. A polarization-matched In_{0.33}Al_{0.67}N/GaN MQW structure was specifically designed by leveraging strain and bandgap. After optimizing the number and thickness of QWs, the 425 nm LED has relative IQE of 62.6% and efficiency droop of only 16.0% at high current density of 333 A/cm². The results indicate that the In_{0.33}Al_{0.67}N/GaN polarization-matched MQW LEDs have great potential in general lighting applications.

ACKNOWLEDGEMENTS

The KAUST authors acknowledge the financial support from KAUST Baseline BAS/1/1664-01-01, KAUST CRG URF/1/3437-01-01.

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