

Design and analytical calculations of the width and arrangement of quantum well and barrier layers in GaN/AlGaN LED to enhance the performance

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Abstract

This research paper discusses an analytical approach to designing the active region of light emitting diodes to enhance its performance. The layers in the active region were modified and the effects of changing the width of quantum well and barrier layers in a multi-quantum light emitting diode on the output power and efficiency have been investigated. Also, the ratio of the quantum well width to the B layer width was calculated and proposed in this research paper. The study is carried out on two different LED structures. In the first case, the width of the quantum well layers is kept constant while the width of the B layers is varied. In the second case, both the quantum well and B layer widths are varied. Based on the simulation results, it has been observed that the LED power efficiency increases considerably for a given quantum well to B layers width ratio without increasing the production complexity. It is also seen that for a desired power efficiency the width of quantum well should be between $0.003 \mu\text{m}$ and $0.006 \mu\text{m}$, and the range of B width (height) should be 2.2 to 6 times the quantum well width. The proposed study is carried out on the GaN-AlGaN-based multi-quantum well LED structure, but this study can be extended to multiple combinations of the semiconductor structures.

1. Introduction

The use of light emitting diodes (LEDs) is increasing day-by-day and brings a new era in lightning. In the coming years, LED-based lighting will be better and cheaper than many other light sources [1]. The LED lighting will be cheap, efficient, and used in many other applications that have yet to be explored. LEDs can provide efficiency in light generation which is much higher than incandescent light bulbs [2]. The efficiency of some of LEDs is close to the theoretical limit of electricity to light conversion set by physics [3]. As LEDs will become the dominant light source over the next decade, the reduction of energy used, and greenhouse gases emitted will benefit everyone [4].

In order to achieve the goal of increasing the efficiency and output power of LEDs, there are various materials and structural engineering-based methods and LED structures that are in use today which are based on multi-quantum wells (MQWs). Most of the reported structures in literature are based on the MQW layers having identical width of the quantum well (QW) and the barrier (B) layers within the structure. For instance, the structure reported in Ref. 5 is a three-layer MQW GaN/InGaN LED. In this structure, the QW width is of 6 nm and the B layer width is of 15 nm. There are also MQW structures [6–8] having three and four layers of QW, respectively. Out of many specifications, there is one thing which is common in all these structures. It is the identical width of all QW layers within a structure, although it is not identical for two different LEDs structures [6–8].

Techniques in trends to achieve the goal of increasing efficiency of optoelectronic devices are based on numerical

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analysis, machine learning, and existing conventional methods. There is a LED [9] which is a five-layer device of GaN in which the author used the machine learning technique to optimize the related algorithm for a GaN-based LED to increase the efficiency. Similar technique is also used [10] to enhance the performance of opto-electronic devices. The author enhanced [11] the performance of green LEDs by using the methodology based on a numerical analysis of structural engineering.

With the same topic of increasing efficiency, this paper investigates the effect of a device design on power output and power efficiency. After the analytical analysis, the ratio of QW to B layers width is proposed which will enhance the efficiency of the device without increasing the complexity and any additional fabrication cost of the device. The work is divided into two cases. In the first case, the QW layers width is kept constant and the B layers width is varied. Whereas in the second case, both the QW and B layer widths are varied. The effects of varying the QW and B layers are investigated and analysed in the structure design proposed in Fig. 1.

In Fig. 1, an attempt was made to modify the width of QW and B layers present in the active region, details of which are provided in the following sections. The importance of doing this work is that in addition to conventional applications of LEDs, the UV LEDs are in use in many fields, as well. UV LED is especially useful for curing purposes in the paper and wood coating industries and is more energy-efficient, dissipates very little heat, contains no mercury, and can be manufactured with a much smaller footprint and far better optical design than traditional UV lamps. In addition to this, UV-LEDs are also used for water treatment [12]. The rest of the paper is organized as follows. In section 2, a brief overview of the QW structures is given. The proposed designs are presented in section 3. The results and discussion are presented in section 4, followed by section 5 in which a comparison of optical characteristics of the proposed designs with the existing ones is presented, and the conclusions are presented in section 6.

2. Proposed methodology

The proposed design considered the following parameters:

1. The minimum width (height) of B is more than twice the width of QW because the width less than this does not make a significant QW. This has been verified by simulating many designs and this condition holds good for all designs reported in this paper, as well as for the previously reported designs in literatures.
2. The width of the last barrier (B) layer (in the case of four QW, the fourth B layer) is either equal or larger than other B layers. As the configuration other than this arrangement generates less output power, the power efficiency of the device obtained is also lower. This condition is also verified on multiple designs. The reason is as follows: since the fourth layer is the widest B layer of all the layers, all the tunnelled carrier gets accumulated in the last well and cannot pass through it.

Steps followed for the simulation:

1. In serial numbers I–V in Table 1.1 the width of all four QWs is kept constant and equal to $0.003 \mu\text{m}$ whereas the width of all four B layers is kept constant and equal but varies from $0.007 \mu\text{m}$ to $0.018 \mu\text{m}$, respectively.
 2. In serial numbers VI–X in Table 1.1 only the last (fourth) B layer is kept constant and wider ($0.06 \mu\text{m}$) than rest three QW layers. Likewise point (1), the width of three B layers is kept equal and varies from $0.007 \mu\text{m}$ to $0.018 \mu\text{m}$.
 3. In serial numbers XI–XV in Table 1.2 also the width of all four QW layers is constant and equal and is kept as $0.006 \mu\text{m}$, whereas the width of B layers varies from $0.0013 \mu\text{m}$ to $0.036 \mu\text{m}$.
 4. Similar to point 2, in serial numbers XVI–XX in Table 1.2 the width of the fourth B layer is kept constant = $0.078 \mu\text{m}$, but wider than the rest three B layers. The range of variation of the first three B layers is from $0.0013 \mu\text{m}$ to $0.036 \mu\text{m}$.
- All these scenarios are tabulated in Tables 1.1 and 1.2.

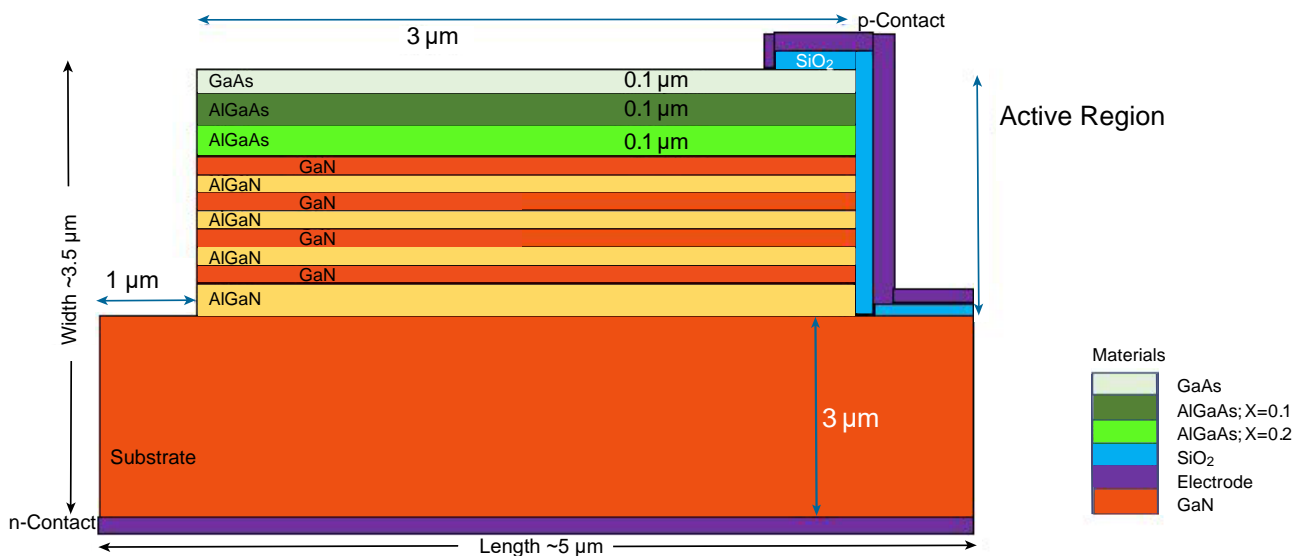


Fig. 1. Schematic design of the GaN MQW LED structure.

5. Some more designs are recorded in Table 2 in which the width of QW2 to QW4 is taken with respect to QW1 layer. The width of QW1 has been fixed and the width of QW2 to QW4 is taken as 10% of QW1, then, 20% of QW1, and so on until 100% (QW1=QW2=QW3=QW4). In this case, the effect of changing the QW layer is studied as opposed to the previous case in which the variability of B layers was investigated. The improvement in the result is quite significant when the width of QW1 changes.

The TCAD tool has been used for simulation of the proposed design of LEDs, as well as their characteristic curves.

Limitations of the proposed design:

- Experimental verification is not done because it requires actual fabrication of multiple designs which is a very costly and time-consuming process.
- Although the experiment is performed on a GaN-based MQW-based LED, it is believed that it will satisfy other LED semiconductor structures, as well.
- The number of QW in the design on which experiments are carried out is four QW designs, but the same approach may be applied to designs having three or five QWs.

Advantages

- There could be multiple ways to enhance the efficiency and increase the optical power of a device, but the proposed method is quick, economic, and efficient.
- Complexity of the device will not get affected after the suggested changes.
- The selected value of QW and B, holding good for (1) to (4), generates the more useful output power and enhanced power efficiency compared to other multiple designs simulated in the paper. It is economic, but efficient.

The same details are also explained with the help of the flowchart shown in Fig. 2, Table 1.1, Table 1.2, and Table 2 are designed based upon the flowchart given in Fig. 2.

3. Structural specification and optical outcome of the proposed design

This section contains dimensional details and results. Many structures are designed and tested in order to conclude the results. In this article, the region under consideration is the active region of the LED device. Remaining regions (layers) and all parameters such as doping, chemical composition, and physical dimension are kept constant and identical for all the simulated designs (structures), since only differences in the width of QW and B layers are investigated in this article. Physical dimensions which are constant and identical in all designs reported in this paper are as follows. The length of the LED device is chosen as of 5 μm, and the width is of 3.5 μm also marked in Fig. 1. The length of all layers apart from the substrate in the LED design is uniform and taken as of 3 μm. The width of the substrate region is of 3 μm with an n-type doping concentration of $2 \times 10^{18} \text{ cm}^{-3}$.

For ease of understanding and clarity, the variation in QW and B dimensions for all respective designs reported in this paper is given in Table 1.1, Table 1.2, and Table 2. Since the active region is an intrinsic region, hence no doping is required. Active region is a junction area sandwiched between p and n region. There are three layers above the active region. The thickness of Al_{0.1}Ga_{0.9}N is of 0.1 μm with a p type dopant having a concentration of $2 \times 10^{20} \text{ cm}^{-3}$. The next layer above this is of 0.1 μm with Al_{0.2}Ga_{0.8}N doped with a p-type dopant having a concentration of $2 \times 10^{20} \text{ cm}^{-3}$, and the topmost layer is of GaN and it is 0.1-μm thick and doped with a p-type dopant having a concentration value of $2 \times 10^{20} \text{ cm}^{-3}$. The anode and cathode electrode contacts are attached as shown in Fig. 1.

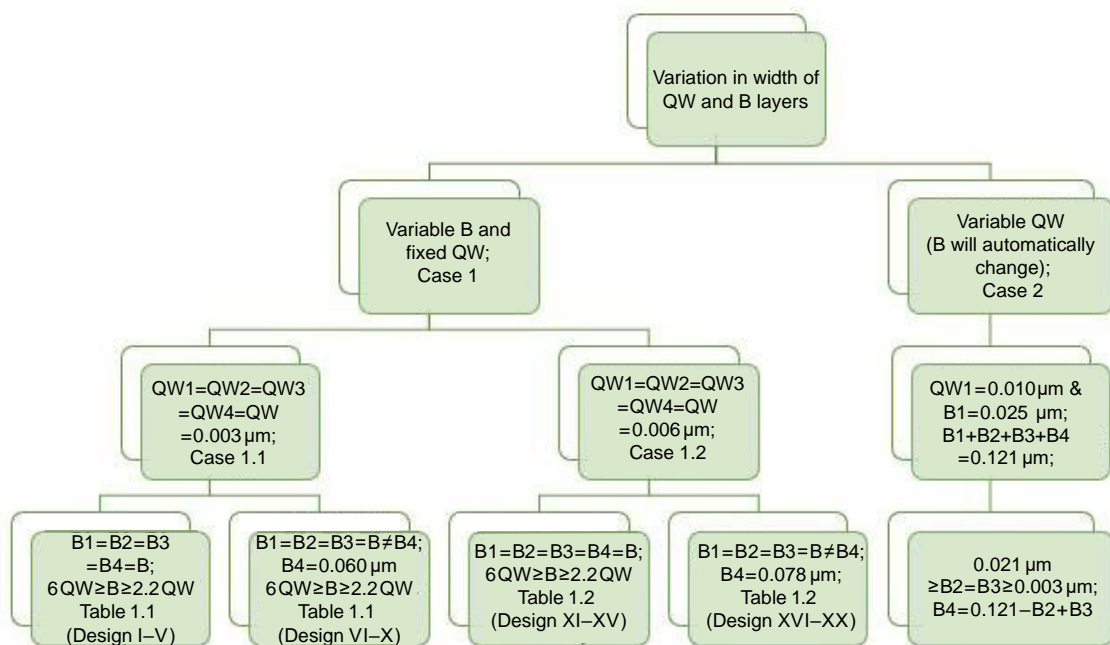


Fig. 2. Flowchart of the proposed design.

Table 1.1.
Dimensional details of the active region with variable B width and constant QW width.

B layer→ Serial no.↓	QW1=QW2 =QW3=QW4 (μm)	B1 (μm)	B2 (μm)	B3 (μm)	B4 (μm)	Width of active region (μm)	Optical power I (mW)	I (mA)	% Power efficiency I (η)
I	0.003	0.007	0.007	0.007	0.007	0.040	1.204	1.450	20.75
II	0.003	0.009	0.009	0.009	0.009	0.048	1.586	1.431	27.70
III	0.003	0.012	0.012	0.012	0.012	0.060	2.005	1.419	35.32
IV	0.003	0.015	0.015	0.015	0.015	0.072	2.228	1.413	39.41
V	0.003	0.018	0.018	0.018	0.018	0.084	2.369	1.402	42.24
VI	0.003	0.007	0.007	0.007	0.060	0.093	3.148	1.429	55.07
VII	0.003	0.009	0.009	0.009	0.060	0.048	3.050	1.427	53.43
VIII	0.003	0.012	0.012	0.012	0.060	0.108	2.973	1.421	52.30
IX	0.003	0.015	0.015	0.015	0.060	0.117	2.859	1.416	50.47
X	0.003	0.018	0.018	0.018	0.060	0.126	2.786	1.405	49.57

Table 1.2.
Dimensional details of the active region with variable B width and constant QW width.

B layer→ Serial no.↓	QW1=QW2 =QW3=QW4 (μm)	B1 (μm)	B2 (μm)	B3 (μm)	B4 (μm)	Width of active region (μm)	Optical power I (mW)	I (mA)	% Power efficiency I (η)
XI	0.006	0.013	0.013	0.013	0.013	0.076	2.865	1.370	52.28
XII	0.006	0.018	0.018	0.018	0.018	0.096	3.061	1.339	57.15
XIII	0.006	0.024	0.024	0.024	0.024	0.120	3.015	1.303	57.84
XIV	0.006	0.030	0.030	0.030	0.030	0.144	2.865	1.262	56.75
XV	0.006	0.036	0.036	0.036	0.036	0.168	2.721	1.215	55.98
XVI	0.006	0.013	0.013	0.013	0.078	0.141	3.659	1.367	66.91
XVII	0.006	0.018	0.018	0.018	0.078	0.156	3.409	1.336	63.79
XVIII	0.006	0.024	0.024	0.024	0.078	0.174	3.141	1.294	60.68
XIX	0.006	0.030	0.030	0.030	0.078	0.192	2.914	1.248	58.37
XX	0.006	0.036	0.036	0.036	0.078	0.210	2.735	1.200	56.97

The dimension and concentration of these three layers will remain constant for all the designs.

Next, the design and width of QW and B layers reported in this paper are discussed. In Table 1.1, the width of QW layer (GaN) from serial number I to X is taken to be of 0.003 μm and from serial number XI to XX (Table 1.2) is of 0.006 μm.

Designs reported in Table 1.1 and Table 1.2 deal with the variation of B layers keeping the width of QW fixed. To evaluate the performance of the designs, power efficiency of all designs is calculated analytically by using the following relation:

$$\eta = \frac{P_{out}}{VI}, \quad (1)$$

where P_{out} is the total power radiated by the LED and VI is the input electrical power supplied to it. The obtained results are compared with the existing designs. Dimensional details of designs under case 1 are divided into two tables for better understanding of different scenarios and are presented as Table 1.1 and Table 1.2

The study of case 1 is divided into two parts which is as follows: first, the width of all B layers is kept identical and varied twice the width of the QW layer to six times the width of QW layer for designs from serial number I to V (Table 1.1) and XI and XV (Table 1.2). And for serial numbers from VI to X (Table 1.1) and XVI to XX (Table 1.2), the width of the fourth B layer (B4) is kept higher than other three B layers (B1, B2, B3).

Here, the schematic representation of only one design, of which simulation results are encouraging, is presented in Fig. 3 as design number XVI in Table 1.2. In this design, the width of all four QW layers (GaN) is of 0.006 μm and the width (height) of all first three B layers (AlGaIn) is of 0.013 μm, whereas the width of B4 is taken to be of 0.078 μm. The remaining dimensional details of all designs in case 1 have already been shown in Table 1.1 and Table 1.2.

The next is case 2 in which both the width of QW and B layers are variable. Since the width of the B layer depends upon the width of QW, as the width of QW changes, the B layer width will change accordingly.

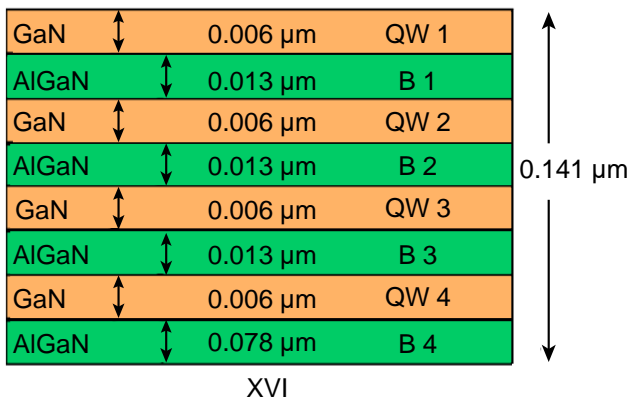


Fig. 3. Snapshot of the designed active region.

As in case 1, the dimensional details of all case 2 designs are given in Table 2. In this case, the width of QW1 is taken as of 0.010 μm, B1 as of 0.025 μm, whereas the combined width of B layers (B1+B2+B3+B4) for all designs is of 0.121 μm.

However, for comparison purposes, some structures with identical widths are also designed and simulated. But as the obtained simulated results and analytical calculated values are not much impressive, they are not presented in this article.

Here, the width of the last three QW layers varies from 10% to 100%, whereas QW1 is kept constant (hence, B1 is

also constant) in all designs in case 2. On the other hand, B2, B3, and B4 are varied accordingly to QW2, QW3 and QW4, respectively. In all designs, B is always kept more than twice the width of QW. As in case 1, in case 2, the width of the active region is not constant.

In addition to the above, two other designs are also simulated in which the arrangement of QW layers is made in such a way that they are non-identical within the structure as much as possible, while keeping B constant and identical for all designs.

The design results were presented in Fig. 4 and the effect of width changes on output power and power efficiency was analyzed and compared.

Here, the obtained output power is of approx. 3.659 mW and power efficiency is calculated analytically using Eq. (1). As the variation of the anode current is not high for all designs, therefore, a value of ~1.5 mA is assumed and the applied voltage is kept at 2–4 volts. In case 2, in which both the QW and B layers of the active regions are variable, and the width of the active region is also not constant, ten structures are tested and simulated, as ten structures are enough to cover this scenario. It is obvious from the simulation results that the structure number V is better in terms of delivering the useful output power and the power efficiency among all other designs in case 2. The next section contains design details, i.e., the identified QW and B ratio.

Table 2. Dimensional details of the active region with variable QW width and B width.

Serial no.↓	QW2=QW3=QW4 (μm) (x% width w.r.t.1 st QW)	B2=B3 (μm)	B4 (μm)	Width of active region (μm)	Optical power 2 (mW)	I (mA)	% Power efficiency 2 (η) (case 2)
I	0.001 (10%)	0.003	0.090	0.134	1.591	1.401	26.13
II	0.002 (20%)	0.005	0.086	0.137	2.776	1.412	37.62
III	0.003 (30%)	0.007	0.082	0.140	3.404	1.421	40.53
IV	0.004 (40%)	0.009	0.078	0.143	3.733	1.426	42.30
V	0.005 (50%)	0.011	0.074	0.146	3.903	1.427	44.40
VI	0.006 (60%)	0.013	0.070	0.149	3.903	1.421	43.23
VII	0.007 (70%)	0.015	0.066	0.152	3.873	1.418	43.08
VIII	0.008 (80%)	0.017	0.062	0.155	3.824	1.411	42.81
IX	0.009 (90%)	0.019	0.058	0.158	3.811	1.407	42.33
X	0.010 (100%)	0.021	0.054	0.161	1.591	1.391	26.13

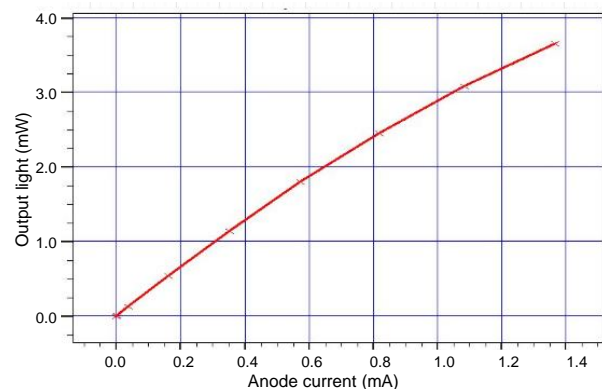
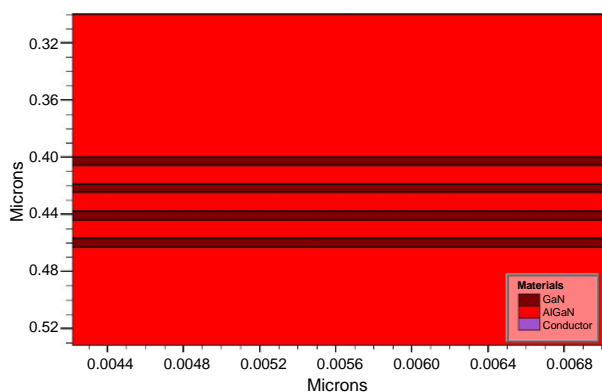


Fig. 4. Snapshot of the active region and the output power vs. current (Case 1.2 structure XVI).

Table 3.
Comparison of the performance of the existing and proposed LED structures.

Structure type	Semiconductor material (QW/Barrier)	Width (QW/B)	Voltage range	Output power	% Power efficiency (η)
MQW structure (4-layer device) proposed design	GaN/AlGaIn	6 nm/13 nm, 78 nm (B4*)	2–4 V	3.65 mW	66.91
MQW structure (5-layer device) [13]	InGaIn/GaN	3 nm/14.4 nm	2–4 V	1.60 mW	41.09
MQW structure [14]	InGaIn/GaN	2.5 nm/6.5 nm	2–4 V	0.87 mW	32.14
MQW structure [15]	III-Nitride	3 nm/17 nm	2–4 V	1.70 mW	44.21

4. Results and discussion

The structure in which the design patterns of QW and B satisfy the empirical relation [(2)–(4)] proved to be better in terms of power efficiency and output power. Relations (2)–(4) concern four QW GaN/AlGaIn-based LEDs, but they should satisfy other semiconductor MQW structures, as well.

$$QW1 = QW2 = QW3 = QW4 \quad (2)$$

$$B1 = B2 = B3 < B4 \quad (3)$$

$$\frac{QW1}{B1} = \frac{QW2}{B2} = \frac{QW3}{B3} > \frac{QW4}{B4} \quad (4)$$

$$\frac{QW1}{B1} \leq \frac{1}{2.2}K \text{ and } \frac{QW4}{B4} \leq \frac{1}{5}K \quad (5)$$

where K is the constant, generally ≈ 1 . The meaning of the design pattern is that if the active region composed of four layers is designed by using relations (2)–(5), the performance of the device is possibly the enhanced version of its previous versions. With the best of our knowledge, no such empirical relation is mentioned in the existing literature. In the next section, a comparison between the performance of the existing design and the proposed design is made.

5. Comparison of optical characteristics of the proposed design with existing designs

As shown in Table 3, the existing MQW design generates less power compared to the proposed design. Although all the reported structures are MQW designs, the number of QW layers in the active region may differ, but still the amount of power generated by the proposed design is high. First, in a MQW structure, if the width of QW and B layers satisfies the proposed relations (2) to (4) and the remaining properties and conditions are identical, then the useful output power and power efficiency of the designed device is higher. Second, though the model is derived by considering a GaN-based LED, the proposed modelling is independent from materials used for the design. The proposed model will be applicable to all semiconductor LED structures having MQW. Literature [13–15] justifies the statement, as well. InGaIn/GaN-based LED [13] is a

five-well structure, the LED described in Ref. 14 is a MQW structure-based LED, and the Indium-based MQW LED [15] all have similar conditions to the proposed GaN-based LED, but the generated output power and power efficiency are lower as compared to the proposed GaN-based LED. Hence, it is justified that the proposed study will apply to all LEDs based on the semiconductor with the MQW structure.

6. Conclusions

To enhance the power efficiency of the MQW LED device, the modification of the physical dimension is one of many possible alternatives. It is seen from the reported results that the output power and efficiency of the GaN LED can be increased by critically designing the layers in the active region with a specific dimension. For a given QW to B ratio, the output power and efficiency can be significantly increased. The increased benefit is both economic and simple, as with no significant modification in the existing technology and infrastructure, the performance of the LED is enhanced. Further conclusion from this article based on the GaN structure referred here is that the QW width range between 0.003 μm and 0.006 μm generates better results. The B width should also be 2.2 times to 5–6 times the QW width.

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