Designing Blue-Wavelength Free White Light: A Dichromatic Approach Using Violet and Yellow-Green LEDs

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Abstract

White artificial light is an important aspect of our daily lives as it illuminates our spaces when it's dark allowing us to be productive later in the day. This has transformed our society. However, most white LEDs dominantly contain blue light which can disrupt our sleep cycle and lower the quality of life. Thus, this project aims to tackle this problem by designing a blue-wavelength free white light at a reasonably high efficiency. This will be done using two complementary colored LEDs which are violet and yellow-green LED to obtain a dichromatic white light. The quantum well material investigated is indium gallium nitride with gallium nitride barrier and bulk. Simulations were conducted using the CrossLight TCAD software to better understand the structure and optimize its various parameters. The final emission spectrum of the white light was used to determine the CIE coordinates of the color, and it was x=0.3545 and y=0.3358.

Background and Introduction

Humans are a diurnal species as we are active during the day and inactive during the night. This is a result of the stimulus received through the eyes to the Suprachiasmatic Nucleus (SCN) which is the main circadian pacemaker [1]. The natural light where the sun rises and sets at specific times in the day synchronizes the circadian system with the environment. The strong blue-wavelength present in daylight increases alertness and elevates body cognitive function during the day and as the sun sets, the body transitions into a more relaxed state suitable to maintain the sleep cycle at appropriate times. The specific wavelengths of light that disrupt the circadian system are between 460 nm and 480 nm as it causes acute plasma melanin suppression [2].

However, this is also the dominant wavelength that is present in most white lights because blue light emitting diodes (LEDs) are the most efficient LEDs up to 83% efficient [3]. While blue light can be beneficial at day, lights are mostly switched on at night when it is dark outside which can significantly disrupt the sleep cycle. It can have a persisting effect even a few hours after the lights are switched off which presents a more difficult problem.

There are other alternatives to LED such as incandescent light bulbs and compact fluorescent lamps (CFL). However, LEDs consume about 80% less energy than incandescent light bulbs and about 30% less energy than most fluorescent light bulbs. As we are working towards a more sustainable future, lowering energy consumption is crucial in having lesser energy needs that need to be met by renewable energy sources. LEDs are also more environmentally friendly as they do not emit any hazardous materials, unlike CFLs which contain mercury and require careful disposal. They also have a longer lifespan which makes them a more cost-efficient material [4]. These are some of the many reasons why LEDs are important and why we should focus on further improving them as they are an integral part of our lives.

There are four methods to producing white light: using a blue LED with yellow phosphor, blue LED with green phosphor and a red LED, using RGB LEDs or using a UV LED with RGB phosphors. The methods are in increasing order of color rendering index (CRI) and decreasing order of efficiency. As mentioned earlier, the most dominant wavelength present in white light is the blue wavelength as the first approach is the most common approach due to its high efficiency. The yellow phosphors emit a yellow light when exposed to radiation from the blue light [5].

One of the existing state-of-the-art approaches to this problem is to suppress the blue wavelength and increase the intensity of red and yellow wavelengths which results in a warmer light as can be seen in Figure 1. A problem with this approach is that while minimal there is still a presence of the blue wavelength. Red LEDs are also not as efficient as blue LEDs, so the overall efficiency of warmer lights is lower than the cool white light made from the first method mentioned above.

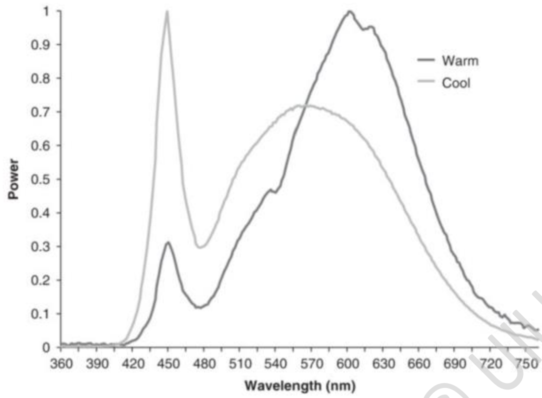


Figure 1: Comparison of the spectrum of warm and cool light [6]

The other approach is to replace the blue wavelength with a violet wavelength, and this is done by the company, Soraa. It also uses two phosphors, green and red to increase the spectral coverage which increases the CRI of the light. The spectral distribution can be seen in Figure 2. However, this is the only commercially available solution and is very expensive. The usage of phosphors also makes it less efficient as the focus of their LEDs is to maintain a high CRI.

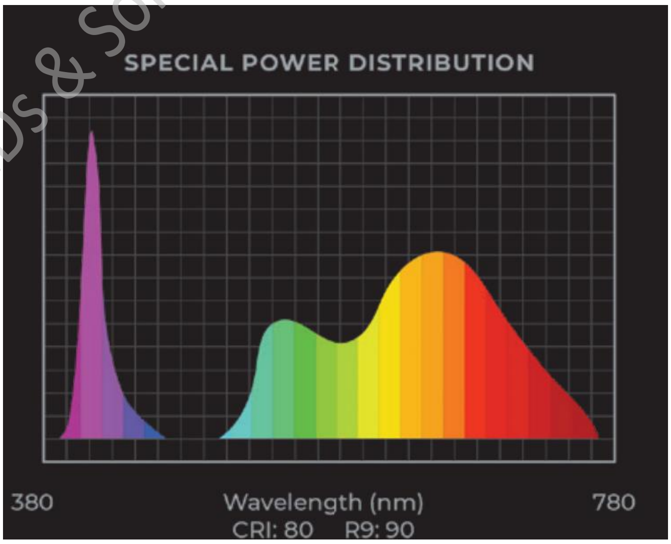


Figure 2: Spectral Distribution of Soraa ZeroBlue LEDs [14]

The design solution that will be explored in this report involves using the violet wavelength of ~ 420 nm to replace the blue wavelength and mixing it with its complementary color of yellow-green ~ 570 nm to achieve a white chromaticity color.

Technical Background:

Light-Emitting Diode

LEDs are made of semiconductors which are materials that can be manipulated to change their electrical conductivity by changing the temperature, optical excitation, and impurity concentration. There are elemental semiconductors which are made from group IV materials such as Silicon and Germanium, binary semiconductors which are made from group III-V materials such as Gallium Arsenide (GaAs), Indium Phosphide (InP) and Gallium Nitride (GaN) or group II-VI materials, ternary semiconductors, and quaternary semiconductors [7]. Semiconductors have a bandgap which is the energy gap between the conduction and valence band and the difference in their energies is the energy required to excite an electron from the valence band to the conduction band.

When two semiconductors of different doping types of the same material are combined, they form a homojunction and when an electric current is used to inject minority carriers it recombines with the majority carriers in the material causing radiative recombination. This results in electroluminescence which is the emission of photons of the wavelength of the material. This is depicted in Figure 3 which also shows that the recombination occurs at the junction [7].

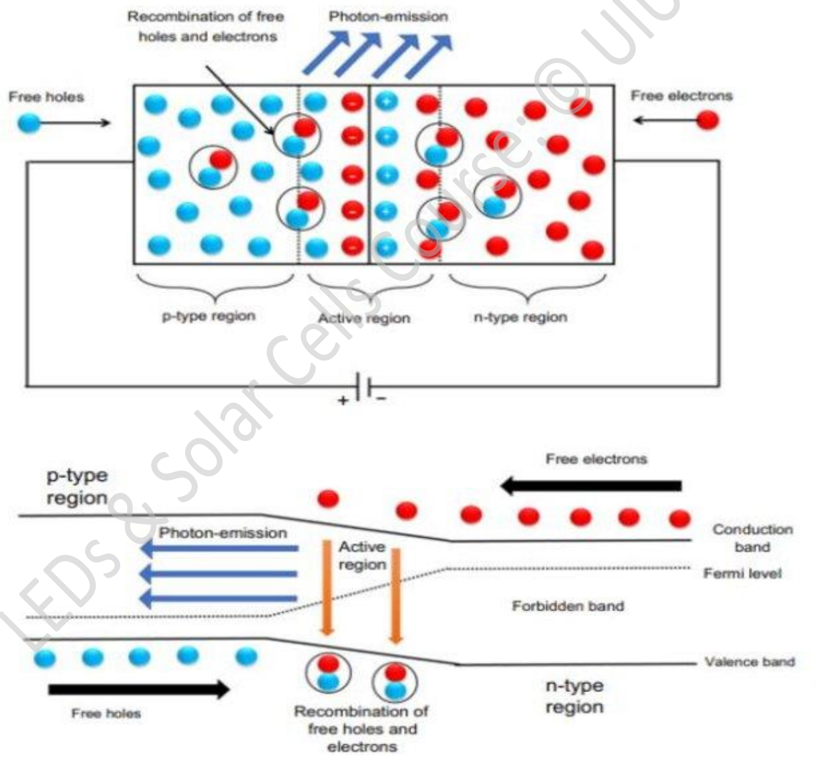


Figure 3: Working Principle of LEDs [8]

The radiative recombination rate is given by [5]:

$$B * \Delta n^2 \tag{1}$$

Where B is the radiative recombination coefficient and Δn is the excess carrier concentration which is given by [5]:

$$\frac{j * \tau_{total}}{q * d} \tag{2}$$

Where j is the current density, τ_{total} is the total carrier lifetime, q is the charge of an electron and d is the combined diffusion length of the minority carriers. The excess carrier concentration term needs to be maximized to increase the radiative recombination rate. A method that is effective in doing that is by introducing quantum wells. Quantum wells confine the area in which radiative recombination is most likely to occur which reduces the d term and thus, increases the carrier concentration as can be seen in Figure 4.

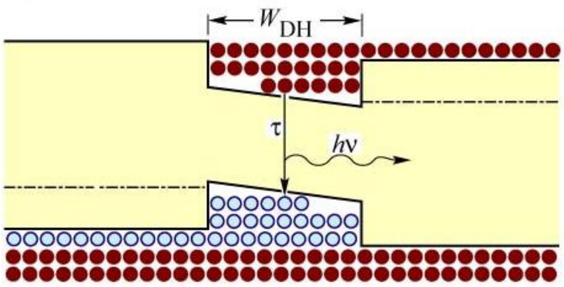


Figure 4: Heterojunction under a Forward Bias [5]

Quantum wells are made by forming a heterojunction of larger bandgap materials on either side of a lower bandgap material. This is a type I band alignment structure. The larger bandgaps form a barrier which can be estimated from the model of a well with infinite barriers. The wave function of a particle in this well would follow the equation below.

$$\varphi_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right) \tag{3}$$

Where A_n is the amplitude of the wave, n is the energy level and a is the width of the well. Using the Schrodinger Equation for the infinite potential in a box, the wavefunction above and the boundary equations, we can solve for the energy of a particle in this quantum well which is given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{4}$$

Where m is the effective mass of the carrier. Real quantum wells, however, have finite barriers which have a lower energy level. The approximation of the energy of the photon emission can be obtained by adding the hole and electron intra-well transition from the 1st level to the ground level and the bandgap of the semiconductor material. A ternary material is usually used as the quantum well material and the bandgap can be obtained using Vegard's Law as shown below.

$$E_g(A_{1-x}B_xC) = (1-x) * E_g + x * E_g(B) - b \tag{5}$$

Where E_g is the bandgap of the respective materials and b is the bowing parameter which shows the deviation from linearity of the bandgap and is a material property.

For this project, the material that is the most suitable is an indium gallium nitride (InGaN) quantum well with GaN bulk and barriers. This is because GaN has a bandgap equivalent to that of in the UV range and the InGaN composition can be modulated to emit a blue-to-green wavelength with a reasonable efficiency. Of course, the green gap is a significant problem in LEDs which is due to the lack of optimal materials with a bandgap in the green range. To use InGaN to emit a green light, the indium composition needs to be increased significantly which decreases the bandgap of the resulting material approaching a green wavelength. The internal polarization field increases with indium concentration due to the increase in lattice mismatch which is not ideal because it significantly tilts the quantum wells and draws the electrons and holes in the wells apart and this is called the Quantum-confined Stark effect (QCSE). To use phosphides which are usually used for red light emission, to emit green light, the large bandgap region of the phosphides has an indirect band gap which results in losses in energy due to requiring the change in momentum of the particles. This loss reduces the quantum efficiency of the device. This is the “green gap” problem.

As the purpose of this design is to create efficient white light from InGaN quantum wells, this problem would have to be addressed. The internal polarization is due to the hexagonal structure of III-Nitride semiconductors. There are two types of induced polarization: spontaneous and piezoelectric. The former is due to the hexagonal structure that lacks crystal symmetry and this polarization in InGaN is depicted by equation 6 while the latter is due to the lattice mismatch between layers of different compositions [5] which is depicted by equation 7.

$$P_{SP} = (1 - x) * P_{SP,GaN} + xP_{SP,InN} \tag{6}$$

$$P_{PZ} = 2\frac{a - a_o}{a_o}\left(e_{31} - e_{33}\frac{c_{13}}{c_{33}}\right) \tag{7}$$

Where a_o is the lattice constant of the material layer, a is the lattice constant of the buffer layer or substrate, $e_{31}$and e_{33} are the elements of the piezoelectric strain tensor, and $c_{31}\ and\ c_{33}$ are the elastic constants of the materials.

The possible solution is to utilize a cubic Zincblende structured GaN instead of the common hexagonal Wurtzite structured GaN. Cubic GaN does not have polarization which increases the quantum efficiency of the device and makes it ideal for this design.

The main criterion used to determine the better parameter is the resulting internal quantum efficiency (IQE) of the device. The internal quantum efficiency is given by the number of photons emitted from the active region per second which is equivalent to the radiative recombination rate over the number of photons injected into the LED per second. This is expressed as,

$$\eta_{IQE} = \frac{B * \Delta n^2}{A * n + B * \Delta n^2 + C * \Delta n^3} \tag{8}$$

where A corresponds to the Shockley-Read-Hall (SRH) non-radiative recombination and C corresponds to the Auger non-radiative recombination. SRH occurs when defects are present in the bandgap which can recombine with carriers and the resulting energy is released to the crystal lattice instead of being released in the form of phonons. On the other hand, Auger recombination occurs when an electron and hole recombine, and the energy released is transferred to a second hole or electron in the conduction or valence band [9].

Auger recombination is especially important because the recombination rate has a cubic dependency and can increase significantly as carrier recombination increases. When the carrier concentration exceeds a certain value, Auger recombination becomes more dominant. Thus, a higher IQE would mean that the carrier concentration is optimized to get a higher radiative recombination rate while having a lower non-radiative recombination rate [9].

Chromaticity

There are three types of cones in the retina of the human eye: the red, green, and blue cones. The perceivable hue of color by these three cones is called the tristimulus values which is made up of X, Y, and Z values for each of the cones. These values can be further simplified and expressed in two values of x and y. The CIE diagram maps this color coordinates to the resulting color perceived which can be seen in the figure below. The 1931 CIE Diagram is the most commonly used chromaticity diagram in the industry. The perfect white or the achromatic point is located at coordinates 0.3, 0.3 but there is a larger white region that has slightly different hues of different colors [10].

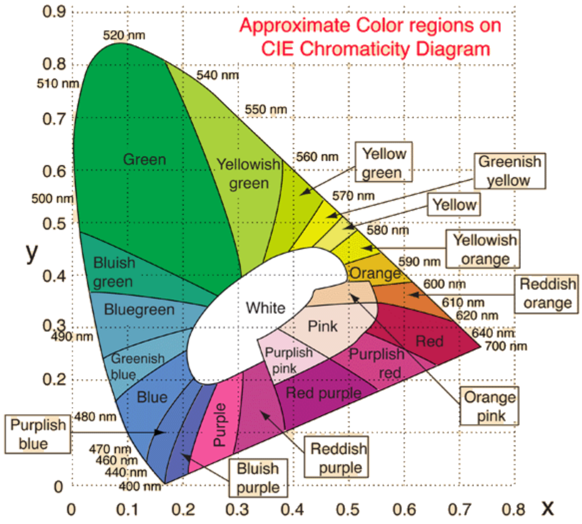


Figure 5: 1931 Chromaticity Diagram

Device design

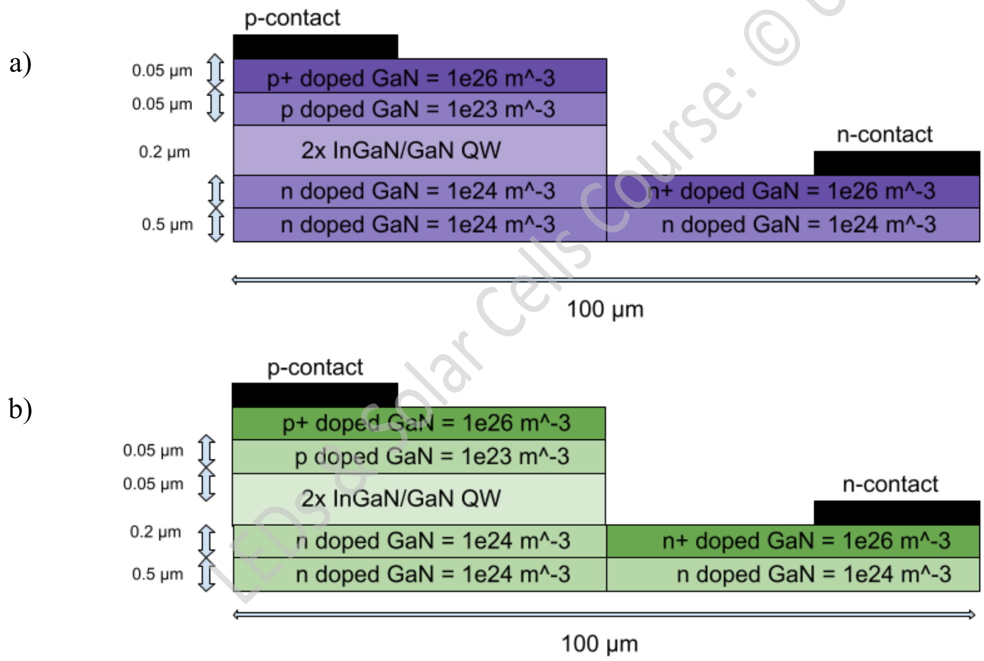


Figure 5: InGaN/GaN Quantum Well LED Device Structure for

(a) Violet LED and (b) Yellow-Green LED

The initial device structure is shown in Figure 5. There is an n-doped GaN and n+- doped GaN to increase the ohmic contact between the bulk layer and contact layer. It is followed by the quantum well structure which includes alternating undoped GaN and InGaN layers, each with 5 nm width. On the other side of the quantum well structure, is a p-doped GaN and p+-doped GaN which again is used to increase the ohmic contact between the bulk GaN layer and contact layer. A mesa of size 50 microns was used to optimize simulation time while also being able to closely represent a regular-sized LED.

To determine the indium concentration required, Vegard's Law was used to estimate a concentration close to what was required. Using the bandgap of GaN which was 3.44 eV, the bandgap of InN which was 1.9 eV, and a bowing parameter of 2.87 eV [11], the composition of InN to achieve a bandgap of 2.95 eV which corresponds to the violet wavelength of 420 nm was 0.177 eV. Using a cubic-GaN bandgap of 3.27 eV [12], the composition of InN to achieve a bandgap of 2.18 eV which corresponds to the yellow-green wavelength of 568 nm was 0.331. However, these values do not include the intra-well energy emission which would mean more indium is needed.

By manipulating the indium content to obtain the desired wavelength, an indium nitride content of 0.125 for the violet LED and 0.367 for the yellow-green LED was obtained.

Simulation and Results

Optimization of the Gan/InGaN structure

The best way to better understand how the device can be optimized is through simulations. The optimization simulation in this project was done using the CrossLight TCAD software. The modulation of each characteristic and its respective effect on the device, especially the internal quantum efficiency was determined. The device also performs differently in different current regions. A rough estimate of the intensities required to produce white light shows that about a 1:5 ratio of yellow-green to violet intensity is needed to produce white light. Thus, the violet LED analysis will focus more on the high current region and droop while the yellow-green LED analysis will focus more on the mid and low current region.

There are many parameters to consider when conducting optimization simulations. The first step was to improve the accuracy of the simulation of the violet InGaN by including the polarization model. As is observed in Figure 6(a), the quantum well tilts because of polarization fields. It can be compared to the band structure of cubic GaN at equilibrium in Figure 6(b) which is not tilted.

a) b)

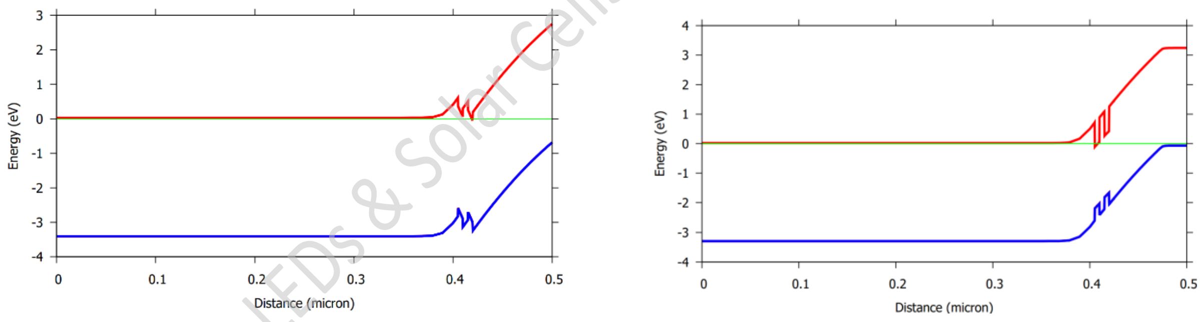


Figure 6: (a) Violet LED Band Diagram at Equilibrium (b) Yellow-Green LED Band Diagram at Equilibrium

I. Manipulating Quantum Well Width

a) b)

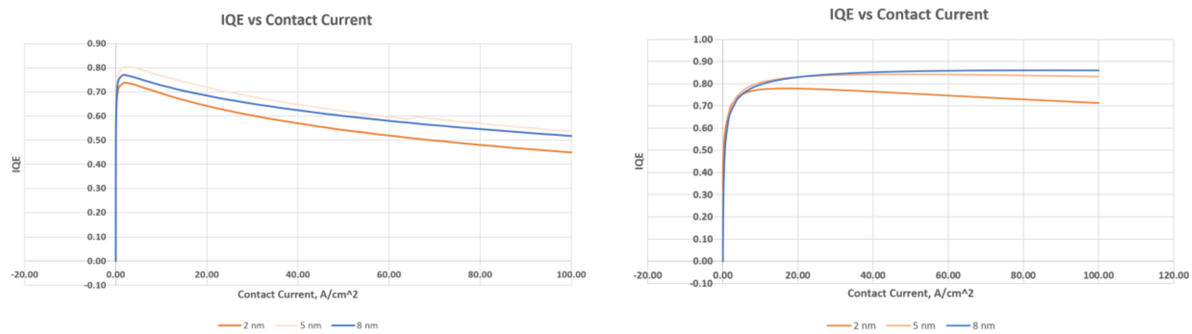


Figure 7: IQE vs Contact Current in (a) Violet LEDs and (b) Yellow-Green LEDs for Different Well Widths

Table I: Values Obtained from the IQE vs Contact Current at Different Quantum Well Widths in Violet and Yellow-Green LEDs

	Violet LED			Yellow-Green LED		
Width, nm	IQE at Peak Current	IQE at Max Current	IQE Droop	IQE at Peak Current	IQE at Max Current	IQE Droop
2	0.7377	0.4493	0.3909	0.7784	0.713	0.084
5	0.804	0.536	0.3326	0.8419	0.8318	0.012
8	0.7699	0.5173	0.3281	0.8602	0.8602	0

When the width of the quantum wells is increased, the capacity of carrier confinement in the quantum well increases allowing more radiative recombination to occur as seen in the relation in equation 1. However, increasing the width of the quantum well can also result in lesser confinement of electrons and thus, a lower concentration of carriers as well as a higher QCSE. This can be observed in the violet LED as the device with 5nm quantum well thickness performs better than the 8nm quantum well. The yellow-green LED, on the other hand, performs better at 8nm due to the lack of polarization effects. However, we can see that the change in IQE from 5nm to 8nm is not as much as the change in IQE from 2nm to 5nm which could be due to the loss in the concentration of the carriers. Thus, the ideal width of the quantum well is 5nm and 8 nm for the violet and yellow-green LED respectively.

II. Manipulating Quantum Well Barrier

a) b)

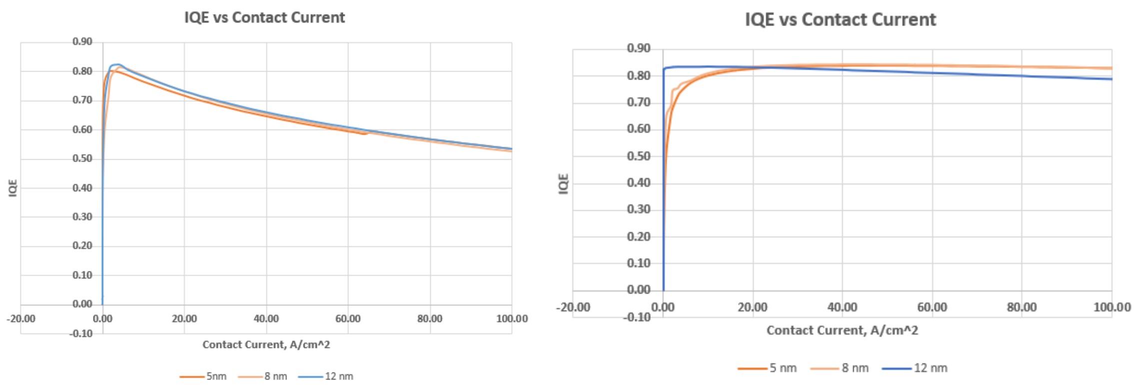


Figure 8: IQE vs Contact Current in (a) Violet LEDs and (b) Yellow-Green LEDs for Different Barrier Widths

Table II: Values Obtained from the IQE vs Contact Current at Different Barrier Widths in Violet and Yellow-Green LEDs

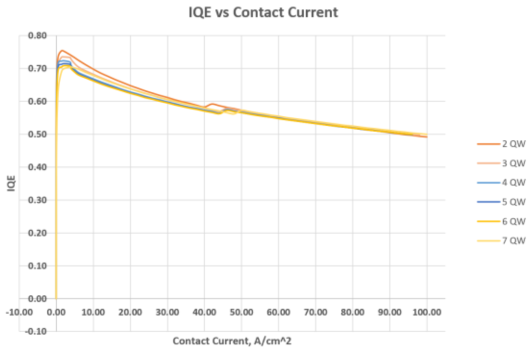
	Violet LEDs			Yellow-Green LEDs		
Width, nm	IQE at Peak Current	IQE at Max Current	IQE Droop	IQE at Peak Current	IQE at Max Current	IQE Droop
5	0.8040	0.5360	0.3333	0.8420	0.8320	0.0119
8	0.8147	0.5230	0.3580	0.8450	0.7130	0.1562
12	0.8255	0.5350	0.3519	0.8370	0.7130	0.1481

Theoretically, decreasing the thickness of the barrier results in a lower electric field within the quantum well which decreases the potential within the well and thus, the kinetic energy of a particle in a well [13]. This can allow more carriers to be captured which reduces the electron leakage. This is observed in the efficiency droop values at each barrier width as the lowest efficiency droop occurs at the lowest barrier width. Thus, the ideal barrier width for both the violet and yellow-green LED is 5nm.

III. Manipulating Quantum Well Number

Another important characteristic to manipulate is the number of quantum wells. As mentioned before, increasing the width of the quantum well reduces the confinement of the carriers. However, increasing the number of quantum wells would result in having more active layers without reducing confinement. Thus, the better method of increasing the active layer in the LED is generally by increasing the number of quantum wells. The limit here would be the increase in complication during the manufacturing process that comes with increasing quantum wells which can make the device more expensive. Thus, the optimal number of quantum wells is determined by how much the internal quantum efficiency increases with the number of quantum wells and if it is significant enough to justify the costs.

a)



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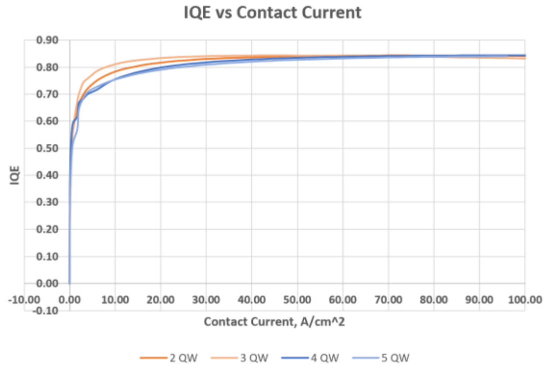

Figure 9: IQE vs Contact Current in (a) Violet LEDs and (b) Yellow-Green LEDs for Different Quantum Well Numbers

Table III: Values Obtained from the IQE vs Contact Current at Different Number of Quantum Wells in Violet LED

Number of Quantum Wells	Peak IQE	IQE at Max Current	IQE Droop
1	0.796	0.463	0.4183
2	0.754	0.492	0.3475
3	0.735	0.497	0.3238
4	0.723	0.498	0.3112
5	0.715	0.499	0.3021
6	0.709	0.5	0.2948
7	0.705	0.5	0.2908

Table IV: Values Obtained from the IQE vs Contact Current at Different Number of Quantum Wells in Yellow-Green LED

Number of Quantum Wells	Peak IQE	IQE at Max Current	IQE Droop
1	0.878	0.793	0.0968
2	0.841	0.831	0.0119
3	0.843	0.841	0.0024
4	0.843	0.843	0
5	0.841	0.841	0

For both the violet and yellow-green LED, the general trend is the decreasing peak IQE while the IQE at maximum current increases with an increasing number of quantum wells. As the change in peak IQE is larger than the change in IQE at max current, the IQE droop calculated decreases with increasing number of quantum wells. When the number of quantum wells is increased, the current leakage experienced decreases as the total width of the active layer increases allowing more confined carriers.

At higher current ranges, a higher number of quantum wells would be ideal as the droop experienced would be lower, and at lower current ranges, a smaller number of quantum wells would be ideal due to the higher peak IQE value.

For the violet LED, quantum wells of 3 and upwards only decreases the efficiency droop by 0.01 for each increase. At 3 quantum wells, a reasonable IQE droop and peak IQE can be maintained which can justify the costs. For the yellow-green LED, having no polarization allows it to operate at much higher current regions and thus, efficiency droop is not observed in this range of current density. In a lower current region, the number of quantum wells that generally have a higher IQE is 3 as can be seen in Figure 9(b). Thus, the ideal number of quantum wells is 3 for both LEDs.

IV. Manipulating Width of p-GaN Bulk

The concentration of doped bulk material is important in providing carriers to be injected into the quantum well. A higher doping concentration in the bulk would result in a higher concentration of carriers in the quantum well at a specific current. This results in a higher IQE as can be seen in equation 8. Increasing the thickness of the doped bulk material also produces similar results. The figure below depicts the higher IQE for a higher thickness of p-GaN over the range of current. However, there is also a more significant droop at larger thicknesses as they roughly converge to a similar IQE at max current. The convergence could be a result of the saturation of the radiative recombination as the excess carriers stop contributing significantly to it. A width of 0.4 μm has an optimal trade-off between efficiency droop and IQE.

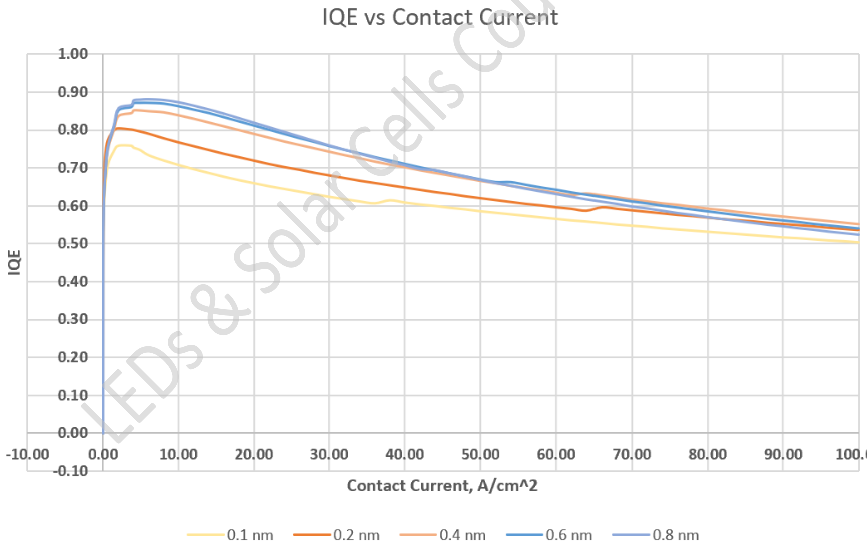

Figure 9: IQE vs Contact Current in Violet LEDs at Different p-GaN Widths

Table V: Values Obtained from the IQE vs Contact Current in Violet LED at Different p-GaN Widths

Width, μm	IQE at Peak Current	IQE at Max Current	IQE Droop
0.1	0.759	0.505	0.335
0.2	0.804	0.536	0.333
0.4	0.852	0.549	0.356
0.6	0.871	0.536	0.385
0.8	0.881	0.520	0.410

Insignificant changes were observed in the yellow-green LED. Thus, the modulation of the width of p-GaN was not simulated in the yellow-green LED.

Final Design

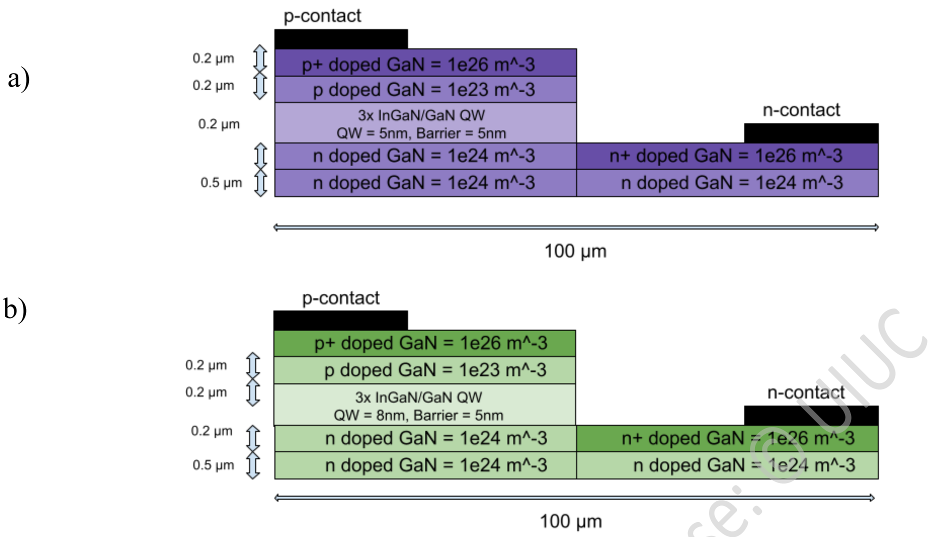

Figure 10: InGaN/GaN Quantum Well LED Device Structure for (a) Violet LED and (b) Yellow-Green LED

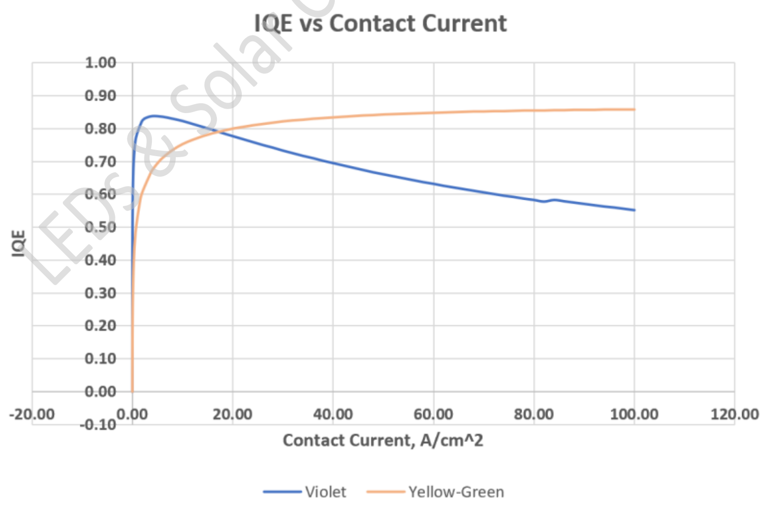

Figure 11: Final Device IQE vs Contact Current

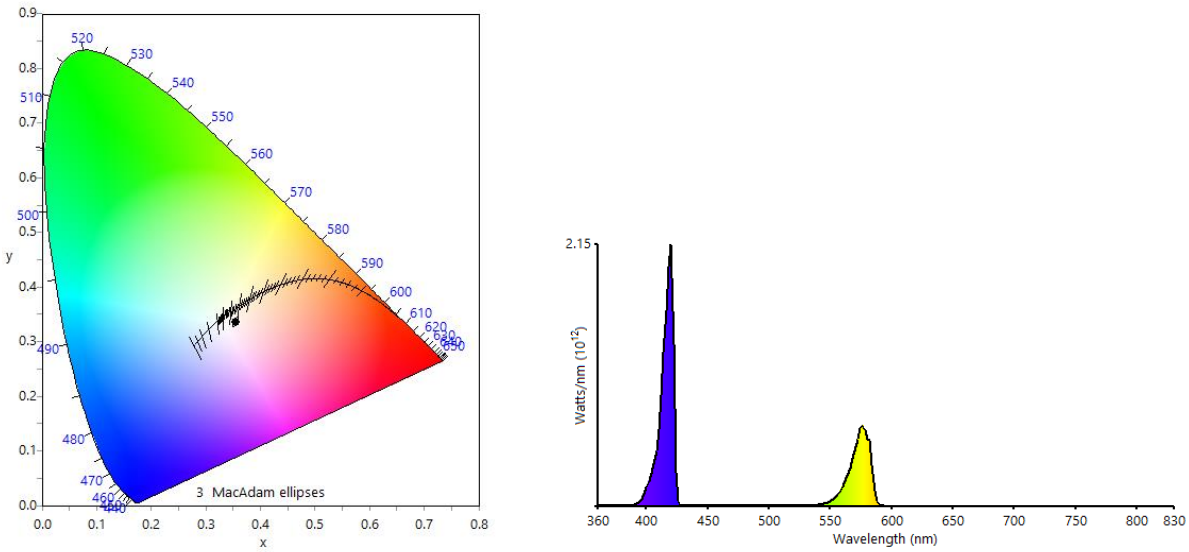

Figure 12: (a) CIE Diagram of Final Device (b) Combined Emission Spectrum

The resulting CIE Diagram obtained using the combined emission spectrum can be seen in Figure 12. The CIE coordinates are x=0.3545 and y=0.3358. The CCT value is 4556 K which is the temperature of the color.

Future work

Reducing Electron Leakage

The current density limit for this simulation was 100 A/cm^2. In this range, little to no leakage was observed as there was no electron concentration on the p-side of the structure. This can also be observed in the band diagrams as the fermi level at the highest current did not exceed the barrier of the wells which would have otherwise significantly increased the probability of occupation of electrons outside the well. It is, however, close to the edge of the barrier and would probably exceed it at higher currents. For a device operating at higher currents, a highly doped p-AlGaN in the range of about 1x10^{20} cm^{-3} can be added between the GaN barrier and p-doped GaN as it has a higher bandgap and can confine the electrons better from leaking into the p-doped side.

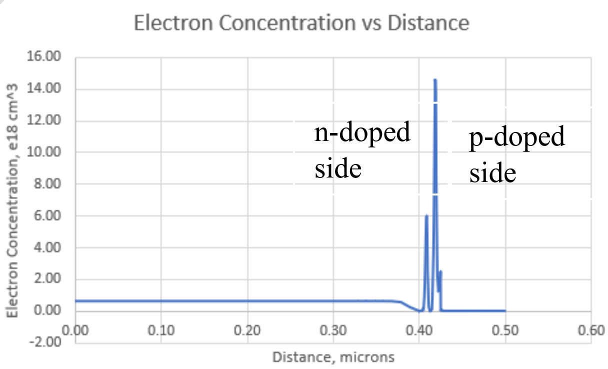

Figure 12: Electron Concentration Plot of Violet LED

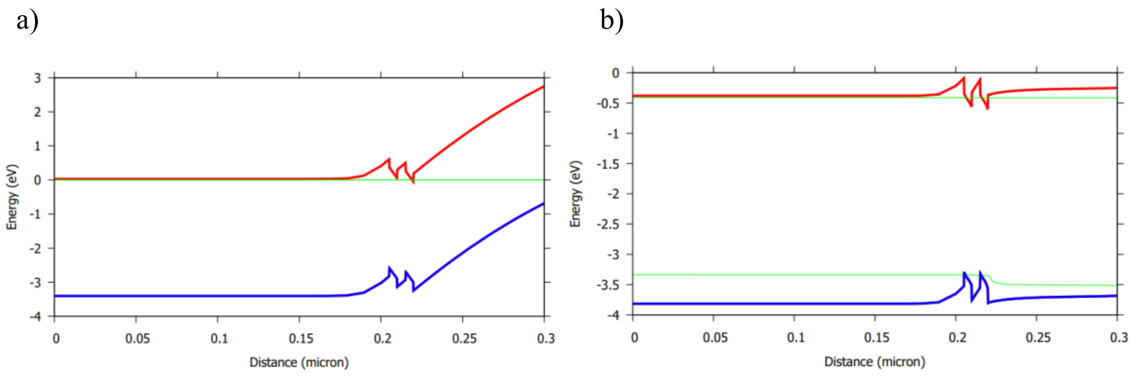

Figure 13: (a) Equilibrium Band Diagram (b) Band Diagram at 100 A/cm^2

Increasing CRI

Dichromatic lights do not have enough spectral coverage to produce light with a high CRI. While it was not the purpose of this project, having a high CRI is important in perceiving the environment around us as a high CRI corresponds to having a more accurate perception of an object. The CRI of an LED can be improved by increasing spectral coverage which can be done by adding phosphors. In the case of this design, red phosphor can be added to make white light with a higher CRI.

Conclusions and Summary

Designing a blue-wavelength free white light is important in enhancing the quality of life as it becomes more prominent in our daily lives. The simulation results produced through the CrossLight TCAD simulation software and OSRAM's color calculator show that it can be feasible to produce white light without the blue-wavelength.

In designing this structure, it was important to optimize parameters such as the quantum well width, barrier width, number of quantum wells, and width of doped layers. It is observed that increasing quantum well width can lead to a larger IQE but is limited by the loss in concentration of carriers. Decreasing barrier width also improves the performance of the device as it decreases the electric field within the well which reduces electron leakage. A higher number of quantum wells increases the active layer without resulting in a loss of confinement but is also limited by the costs associated with the increased number of quantum wells. Finally, the last parameter simulated is the width of the p-doped GaN bulk layer which shows a large increase in IQE peak and a small increase in IQE at maximum current as the width of the p-GaN is increased which can be optimized to produce a higher performing device.

The resulting emission spectrum with white CIE coordinates shows that a dichromatic white light with reasonably high efficiency is possible. However, the CRI of the resulting light needs to be significantly improved before it becomes a more feasible solution. There is also the challenge of the development of cubic GaN which is mostly in theoretical stages, so this is a design solution for the future when cubic GaN becomes cheaper and more commercially available.

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