# Design of Monolithic White LED Using InGaN/GaN/InGaN MQW Structures

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**Abstract**

The goal of this project is to use the Crosslight TCAD software to investigate the possibility of using InGaN/GaN/InGaN multi quantum well structures to output white light from a monolithic entity. By mimicking conventional blue LED + yellow phosphor white light generation, a number of quantum wells will focus on generating blue light and a number of quantum wells will focus on generating yellow light. By changing the parameters and composition of these structures, a tunable color profile of this white LED should be achievable.

## 1 Introduction

It can be said that the discovery of fire was a pivotal step toward humanity's domination of the planet. Fire offered us protection and a method of processing food for better consumption. Another benefit of fire was that it allowed early humans to traverse through the darkness and not be limited by the time of day. For thousands of years, the only way humanity lit up the night was with fire. Though various incremental improvements were made to fuels and to lamps, fire was the major source of light up until the the early 19th century. [1]

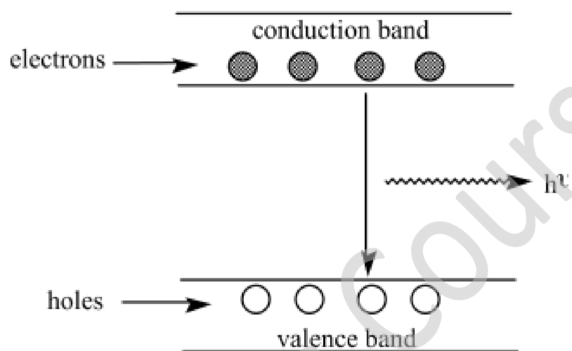
Humphry Dey was first able to demonstrate generation of light from an arc lamp using charcoal rods around 1803. This spurred inventors to improve upon his design; finally culminating in Thomas Edison's research in the conventional incandescent bulb we know today. Unfortunately, due to the power demands of such lighting systems, research moved to florescent bulb technology in the early 20th century. Yet, this too was an inefficient system of lighting. With the world increasingly modernizing, the demand for power and lighting grew. In addition to being inefficient, such systems have lifetimes that are unacceptable as we move to the future. [1]

Enter the Light Emitting Diode. By combining semiconductor physics and the concept of radiative recombination, generation of light was achieved with ”solid-state” devices. While working in General Electric, Nick Holonyak, Jr., invented the world's first visible spectrum LED in the form of red diodes. To this day, LEDs remain the fastest growing and developing lighting technologies. Being able to directly convert electric power to light with no intermediate steps results in large improvements in the lumens per watt produced. Since these structure are solid-state devices, another benefit of LEDs are their long lifetimes. As the world moves toward a more sustainable frame of mind, it is a certainty that the future of lighting technology will continue to be based around LEDs. [1]

Yet, LEDs too have their limitations, most of which revolve around their color accuracy. Since they are a relatively new technology, there exists a large opportunity in improving efficiency and color rendering especially for white light generation. This project uses the Crosslight TCAD software to simulate new LED structures that are able to generate "white" light efficiently from a monolithic device. Such a structure would not require the use of phosphors or require multiple LEDs for white light generation, thereby, streamlining the manufacturing processes.

## 2 LED Physics & Technology

A Light Emitting Diode or LED is a semiconductor light source. Light is released from the structure when electricity flows through the device. This is called electroluminescence. Photons are released by the radiative recombination of electrons and holes. Unlike wide-band sources such as incandescent bulbs, the wavelength of photon released is equal to the energy drop of electron to hole. [2] Thus, LEDs are not white light sources but can be sources of single wavelength light. This makes them highly efficient for colored light applications such as traffic lights.



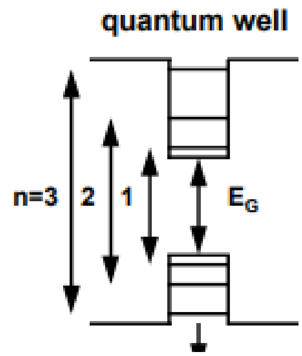

*Source:* Light Emitting Diodes, Edwards, Kimberly D.
Figure 1: Radiative Recombination of Electron-Hole Pairs to Release a Photon of Light

The energy released in a photon, and therefore, the wavelength of photon released can be engineered using quantum structures or quantum wells. A quantum well is a thin layered semiconductor structure in which we can control quantum effects. They derive most of their characteristics from the confinement of carriers (electrons and holes) within them. The method by which a quantum structure can be constructed is by sandwiching a semiconductor material of smaller band gap between semiconductor materials of larger band gap. [3]

We can understand the physics of these quantum wells by looking at Schrodinger's Equation (Equation 1) for a "Particle in a Box". The equation for the $n^{th}$ allowed energy level is as follows:

$$\frac{\hbar^2}{2m}\frac{d^2\phi_n}{dz^2} + V(z)\phi_n = E_n\phi_n \tag{1}$$

The wave equation sets fixed energy states with which electrons can exists inside the quantum well. Thus, the final recombination energy is a summation of the *Band Gap* and the *Energy States* in both the conduction and valence band of the quantum well. This can be visualized as follows:



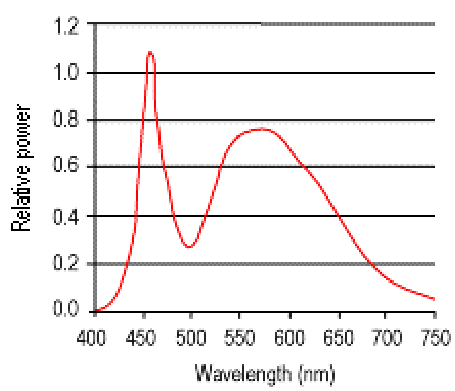

*Source:* Optical Physics of Quantum Wells
Figure 2: Radiative Recombination of Electron-Hole Pairs to Release a Photon of Light

By choosing the band gap of the bulk and quantum well material, the excited photon wavelength is engineered.

## 2.1 State of the Art

Due to their high efficiency, LEDs have disrupted the lighting industry as a whole. One focus in industry is to build ”white” light emitters with a color temperature around 6000K. This is because, sunlight has a color temperature of around 6000K and thus our eyes are naturally calibrated to see the best in this illumination. [4] The spectrum of sunlight that reaches the Earth's surface is close to the idealized blackbody spectrum at 6000K. To our eyes, this is perceived as white light.

Since LEDs are single wavelength light emitters, there are two methods by which we can use LEDs to generate ”white” light based around the idea of color mixing. In additive color mixing, we perceive the color white when red, blue and green light are mixed in equal proportions with each other. This could be done with three LEDs, one for each color but the ”Green Gap” limits the use of such a method. A second method is phosphor aided color mixing in which, a phosphor is used in conjunction with a blue led to generate ”white” light. The phosphor absorbs some of the blue light and emits light in a wide-band yellowish color. Many new phosphors are under research to improve color rendering. [5] A sample spectrum of phosphor-aided ”white” light generation is below:

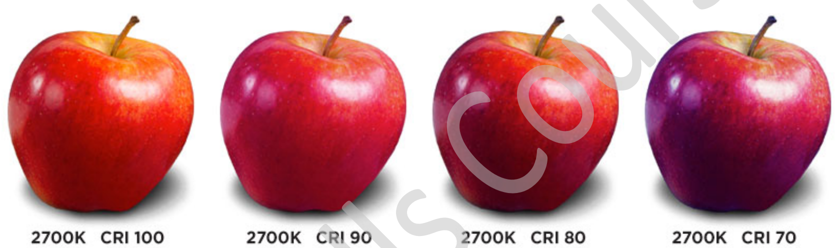



*Source:* How is white light made with leds?
Figure 3: Phosphor Aided ”White” Light

### 2.2 The Problem with ”White” LEDs

The biggest issue with any method of generating ”white” light from solid-state source is the low CRI. CRI or the Chromaticity Index is a method of characterizing light sources by their hue and saturation. In simple terms, the CRI refers to how ”realistically” the source can illuminate and show an object’s color. A CRI of 100 means that the illuminated object’s is color accurate to what it would look like under sunlight. Incandescent bulbs have CRIs over 95 and fluorescent lamps have CRIs about 60 while, ”white” LEDs often max out around 80. [6]

Both ”White” LED technologies have the same low CRI but due to different reasons. RGB color mixing LEDs have low CRI due to the ”Green Gap”. This is a phenomenon in solid-state devices where, an efficient green light source is not yet available. This has the added disadvantage of decreasing the overall efficiency of the ”White” LED. In an effort to not use multiple LEDs and to maintain performance, ”white” light is more commonly produced through the Blue LED + phosphor method. Unfortunately, this method leads to cooler emissions (illuminated objects tend to have a blue tinge) due to the fact that the phosphor emission has poor color rendering. [7] Modifications to get around this issue involve more phosphors or the adding of red LEDs, but this once again drives costs up. Below, is an example of the effect low CRI has on an object from a light source of 2600K.




*Source:* CRI - Color Rendering Index
Figure 4: Effect of CRI on an Object

Due to this color distortion effect, lighting applications prefer not to use low CRI sources. This could be due to aesthetic concerns as in the case of interior design, but could also be due to safety considerations as in the case of automotive lighting systems. Thus, the industry as a whole is working toward new methods that improve CRI.

## 3 Proposed Monolithic ”White” LED

Because of the poor color rendering ability of the phosphors and the presence of the ”Green Gap” in LED devices, white LED topologies suffer from poor CRI. The goal therefore, is to not use phosphor coatings or more than one LED structure. A new topology thereby requires photon emission through electron-hole pair recombination but without green light emission. Hence, the LED must have a blue + yellow emission spectrum like that of the phosphor assisted LED, while being generated from a monolithic structure.

Using the properties of color mixing, a multi-quantum well device could be constructed from which the emission could be gained. In this MQW device, a few quantum wells will focus on blue light emission while the others will focus on yellow light emission. To build such a structure, InGaN and GaN could be used. The band gaps produced by $In_{1-x}Ga_xN$ can produce emissions with a wide range of wavelengths depending on the doping of In. By working with the doping concentration, the height of the barriers of the quantum well and the thickness of the quantum well itself, the color temperature from the emission spectrum could be tuned to whatever is required. The theorized structure therefore is:

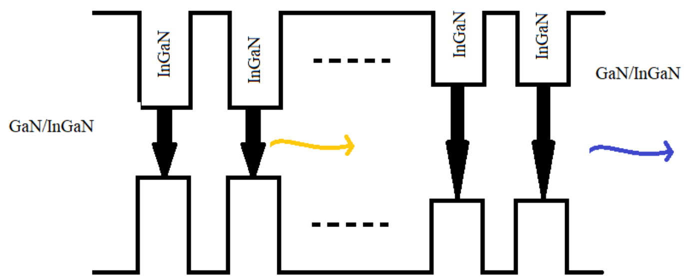



Figure 5: Theoretical Structure of Proposed "White" LED

### 3.1 Device Structure

To get the best color output, an ideal structure would use many quantum wells to maximize the probability of radiative recombination [8]. Unfortunately, more quantum wells leads to larger internal resistance of the structure simply because there is more material for the current to pass through. Because of this, and to also try and minimize simulation time, a design decision was made to work with a three quantum well structure. The well closest to the p-side will focus on blue light emission while the other two will focus on yellow light emission.

The following table describes all the required material properties of wurtzite InN and wurtzite GaN. [9]

Table 1: Material Properties and Values at 300K

| Property | InN | GaN |
|---|---|---|
| Lattice Const. | 3.533 Å | 3.186 Å |
| Band Gap | 0.65 eV | 3.39 eV |
| $m^*_e$ | $0.11m^*_o$ | $0.2m^*_o$ |
| $m^*_h$ | $1.63m^*_o$ | $0.8m^*_o$ |
| Conductivity | $0.666\ \Omega^{-1}\ cm^{-1}$ | $0.5\ \Omega^{-1}\ cm^{-1}$ |
| $\mu_n$ | $250\ cm^2\ V^{-1}\ s^{-1}$ | $440\ cm^2\ V^{-1}\ s^{-1}$ |
| Raditative Recomb. Coeff. | $2\times10^{-10}\ cm^3\ s^{-1}$ | $1.1\times10^{-8}\ cm^3\ s^{-1}$ |

For ease of calculations and simulations, the width of the quantum well is fixed to 10nm. This constrains the "tunability" of the structure in the long run, but aides in finding the material properties. The energy in one photon of light is related to the wavelength by a simple formula. As stated, this energy is the same energy drop experience during a radiative recombination of an electron-hole pair.

$$E\,(eV) = \frac{1240\,(nm\,eV)}{\lambda\,(nm)} \tag{2}$$

Using Equation 2 ($\lambda$ is the wavelength), the energy in a photon of yellow light (assuming wavelength of 580nm) is 2.14 eV while, the energy in a photon of blue light(assuming wavelength of 470nm) is 2.64 eV.

The bowing parameter(b) of InGaN is -1.640 eV. [10] Using the material values presented in the table and equation 3 for Vegard's Law, it is possible to find the composition of In required for blue and yellow emission. Vegard's Law is ubiquitous and therefore can be used (without the bowing) to find whatever parameter is required.

$$E_g(A_{1-x}B_xC) = (1-x) * E_g(A) + x * E_g(B) - b \quad (3)$$

Therefore, we get the following compositions for the blue and yellow quantum wells:

Table 2: Material Properties of the InGaN wells

| Property | InGaN Blue | InGaN Yellow |
|---|---|---|
| Lattice Const. | 3.25 Å | 3.31 Å |
| Band Gap | 2.6383 eV | 2.1379 eV |
| In Concentration | 0.1843 | 0.3670 |
| $m^*_e$ | $0.1834m^*_o$ | $0.167m^*_o$ |
| $m^*_h$ | $0.9530m^*_o$ | $1.1046m^*_o$ |

The energy of the allowed levels in a quantum well is given by equation 4 for an infinite quantum well where, h is Planck's constant, n is the integer level, m* is the effect mass of the carrier in question and L is the width of the quantum well.

$$E_n = \frac{n^2 h^2}{8m * L^2} \quad (4)$$

As stated earlier, this energy adds to the band gap energy for the actual transition experienced. These levels are present for both holes and electrons. Luckily, the energy values gained from this expression are larger than the actual energy shift in a finite quantum well.

Due to the blue shift, caused by the recombination from higher energy levels in the conduction and valence band of each quantum well, the actual amounts of Indium should be increased. Even with higher Indium concentrations, the confinement produced by a conventional GaN/InGaN structure resulted in changing the wide band gap material to $In_{0.05}Ga_{0.95}N$. This eliminates all the unwanted higher energy levels which was causing further blue shift.

Quantum barriers are important since, carriers prefer to recombine by releasing the least amount of energy. Insufficient barrier thickness will not confine carriers in the well and will result in all the recombination releasing yellow photons (since it has the smaller band gap). The quantum barriers between each well will be of 5nm thickness which provides sufficient confinement. The barrier between the two yellow light quantum wells will be GaN. The barrier between the blue quantum well and the first yellow quantum well will be of varying Indium doped InGaN. The height of this quantum barrier is directly related to the amount of carriers that tunnel through. Therefore, the final emission temperature can be tuned simply by changing the height of this barrier. Having more yellow light produced leads to a warmer "white" light and vice-versa.

To increase conductivity of the device, the InGaN bulk has to be doped. The effect of doping on the band structure is another factor that should be taken into consideration. High doping tends to cause band shrinkage which reduces quantum confinement in the edge wells, but low doping causes poor efficiency. For the ease of simulation, the band shrinkage due to doping was not taken into account by the Crosslight TCAD software. Therefore, an equal heavy doping of $1\times10^{22}$ $m^{-1}$ holes was set on the p-side and $1\times10^{22}$ $m^{-1}$ electrons was set on the n-side. The thickness of the bulk was arbitrarily set as 1 micron.

To red shift the emission spectrum, the final composition for the blue quantum wells were experimentally chosen to be $In_{0.26}Ga_{0.74}N$. The composition for the yellow quantum wells were chosen to be $In_{0.38}Ga_{0.74}N$. This highlights a significant difference between the design compositions and the final compositions. If bowing was not taken into account, the design parameters better line up. With a "b" of 0 eV, Equation 3 results in $In_{0.27}Ga_{0.73}N$. This is because, in the "crossligh.mac" file it was found that the bowing parameter and the band gaps of InN and GaN were different (older values) that what was stated above. In order to maintain the file as standard, the necessary modification to the structure and composition of the device was performed.

### 3.2 Simulation Results of Final Structure

To get a neutral white emission, the barrier between the blue quantum well and the first yellow well was $In_{0.01}Ga_{0.99}N$. To produce a cool white emission, this barrier was changed to pure GaN. To produce a warm white emission, the barrier was lowered to $In_{0.02}Ga_{0.98}N$. This was done to allow more flow of carriers into the yellow well, but also maintain confinement in the blue well. The simulations line up well with the assumption that the barrier height and thickness dictate the tunneling and pass-through of carriers from one quantum well to another. hence just with changing Indium doping in this barrier from 0% to 2%, we have control over the color temperature.

Hence, the final structure of the monolithic, neutral emission ”White” LED is as follows:

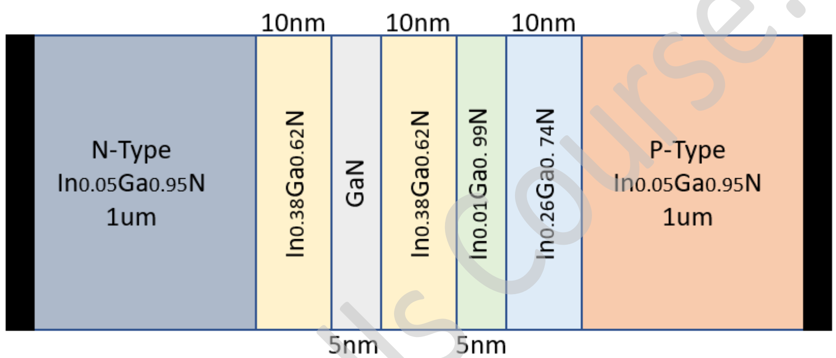



Figure 6: Structure of Monolithic ”White” LED

The Radiative Recombination of the monolithic, neutral emission ”White” LED is as follows:

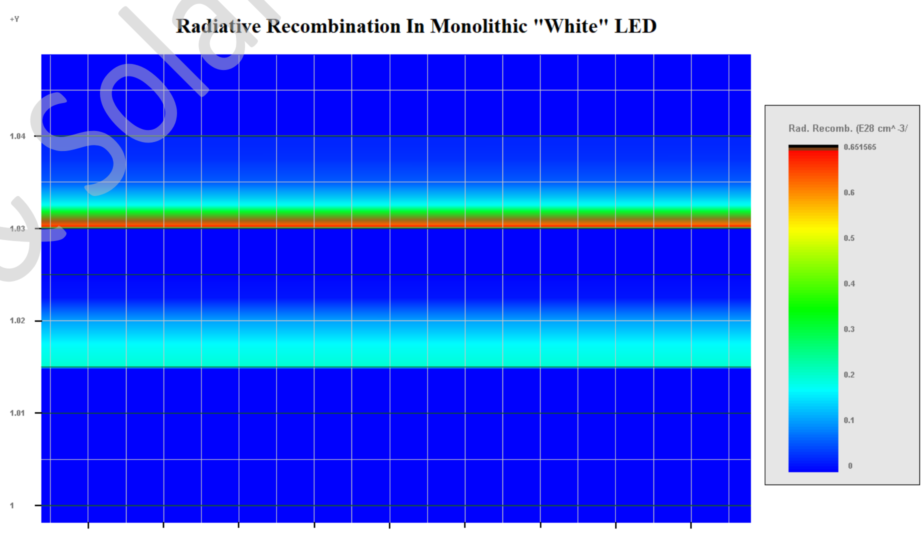



Figure 7: Radiative Recombination In Monolithic ”White” LED

The Band Diagram (0.25$\mu$m around the MQWs) of the monolithic, neutral emission ”White” LED under no bias is:

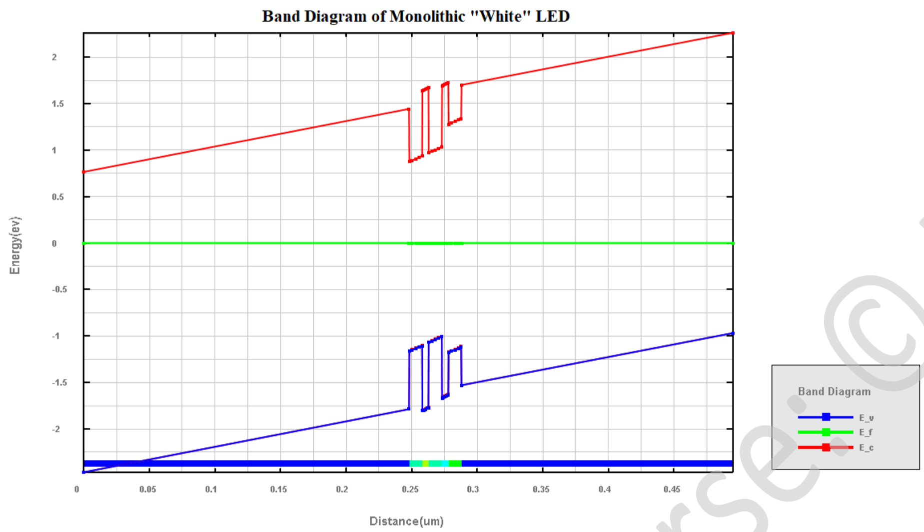



Figure 8: Band Diagram of Monolithic ”White” LED

The Band Diagram (0.25$\mu$m around the MQWs) of the monolithic, neutral emission ”White” LED under forward bias (5A forward current) is:

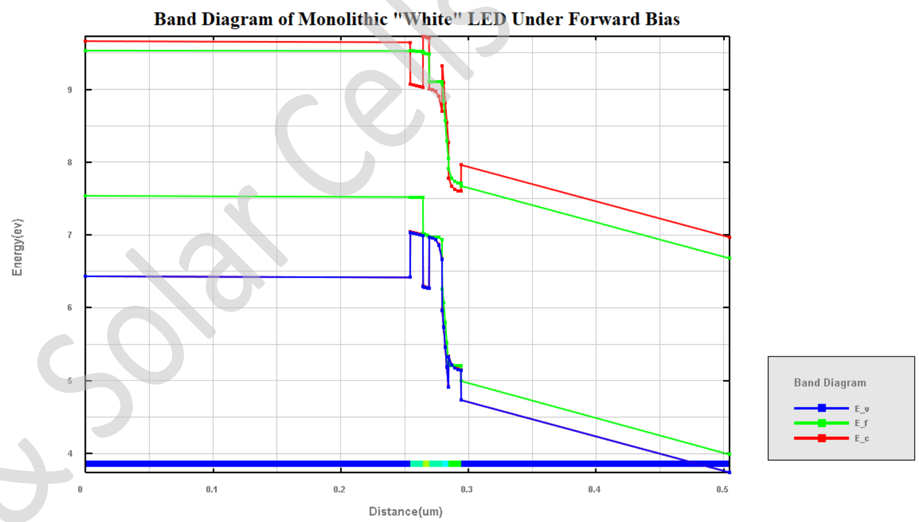



Figure 9: Band Diagram with Forward Bias

The IV Curve and Internal Quantum Efficiency of the monolithic, neutral "White" LED is:

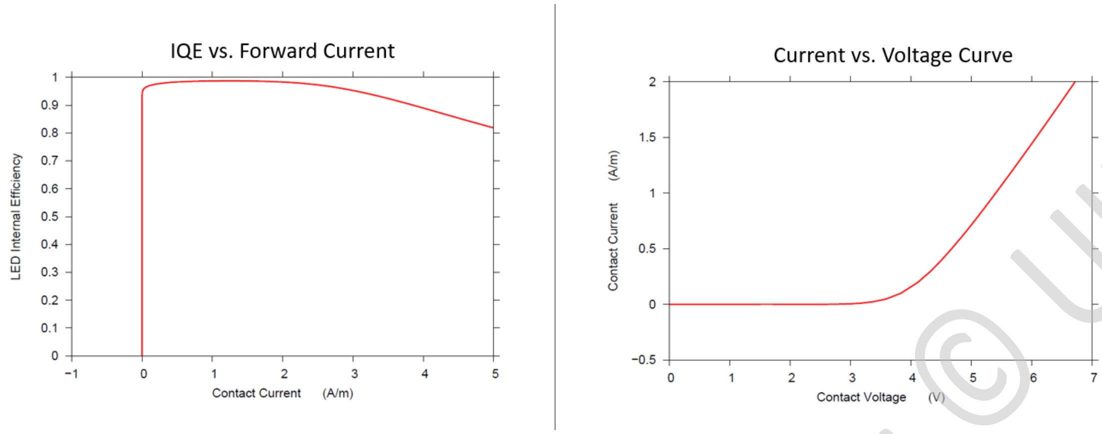



Figure 10: Band Diagram with Forward Bias

The emission spectra for the monolithic, white LED is given below. All three temperatures are plotted on the same graph to highlight the difference between them.

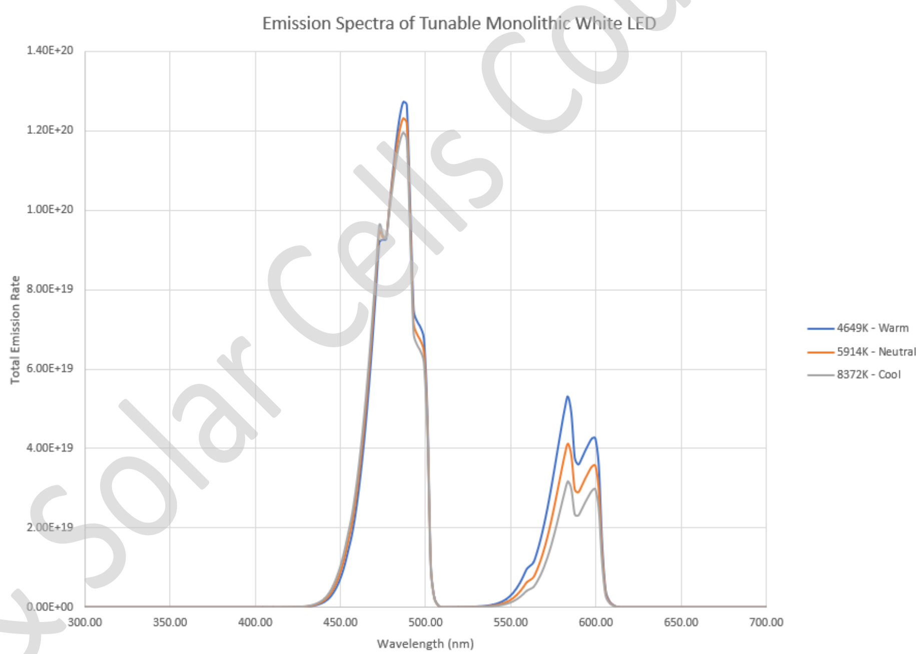
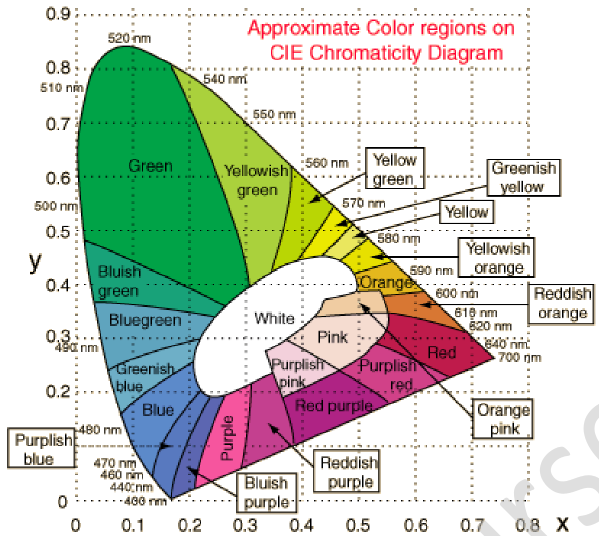



Figure 11: Tunable Emission Spectra

The method by which color accuracy can be measured is through a CIE diagram. [11] The CIE 1931 color space linked the emission spectrum of a source to what is observed by the human eye. The human eye hase three types of cone cells that sense light with peak spectral sensitivity in short ("S", 420 nm 440 nm), middle ("M", 530 nm 540 nm), and long ("L", 560 nm 580 nm) wavelengths. The functions that characterize these responses are known as Tristimulus Functions. By performing an integration and convolutions of a normalized spectrum over these functions, it is possible to extract Tristimulus values. These values (X,Y and Z) can be further normalized to just two dimensions (x and y). Plotting these points onto a CIE diagram gives us a good characterization of the expected color from a spectrum output. The approximate color regions on a CIE diagram are shown below:




*Source:* The CIE Chromaticity Diagram
Figure 12: CIE 1931 Color Regions

Using a Spectrum to CIE converter [12], we are able to plot the chromaticity points for the three different temperatures on a CIE diagram using the GoCIE software. [13]

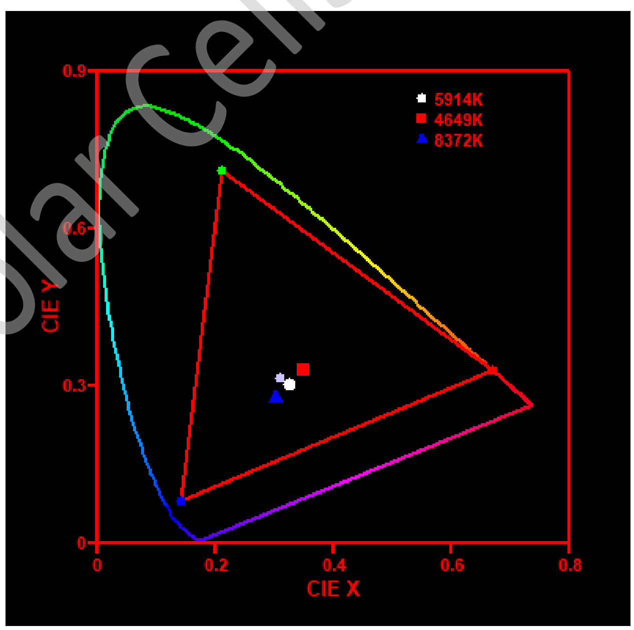


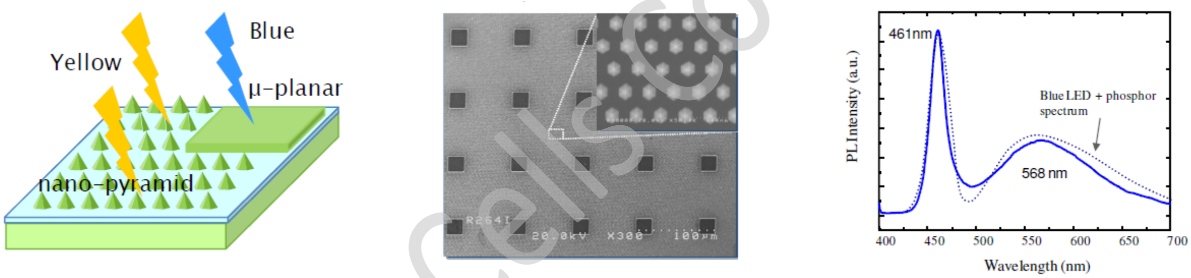

Figure 13: Monolithic "White" LED CIE Plot

We see that the color temperature for the neutral emission ($In_{0.01}Ga_{0.99}N$) is around 5914K (noted by the bigger white dot in the above picture) which is very close to the goal of 6000K (noted by the small gray dot in the above picture). Unfortunately, the exact amount of doping required for perfect white emission was not found. Even though phosphors have lower color rendering ability, they have the benefit of emitting over a wider bandwidth. As of now, the device tends to still be blue shifted. It is to be noted that with the present structure, stronger cyan or greenish emission would help pull the final color toward 6000K white. Phosphors are able to perform this shifting thanks to their spectrum. For this structure, adding a green quantum well was out of the question due to the green gap. So was adding a gradient of wells, as this would increase resistivity.

## 4 Summary & Conclusions

Basic simulation with the Crosslight TCAD software produced encouraging results. From the results and the CIE diagram presented, we see that a monolithic structure has the potential to produce white light. Therefore, the concepts of color mixing and band engineering can be coupled together to construct devices with which manufacturers have greater control over the color temperature.

While perfect 6000K color emission was not possible from the structure presented in this proposal, it must be noted that a lot of design decisions were taken to maximize ”simulatibility”. By opening up these design constraints (well width, barrier width, doping concentration and bulk material), it will become easier to produce better emissions. Firmer grasp of device physics as well as the Crosslight TCAD software would be required to further optimize the device. Luckily, certain research groups have already been able to manufacture similar structures [14] as shown below.




*Source:* White Emission from InGaN Multi-quantum Wells on c-Planes and Nano-pyramids Hybrid Structure

Figure 14: Monolithic ”White” LED in Practice

Another vital characteristic for manufacturing of such devices is the cost associated with InGaN and GaN growth. As of current technology, such materials and semiconductor devices are of high cost making phosphor assisted emission preferential. Even if such a structure could be manufactured, its usefulness to consumers would be severely limited by its cost. Thus, the economics of semiconductor devices must also be taken into consideration for future work.

It is encouraging that 50 years prior, a similar statement could be made about Silicon based semiconductor devices. Since then, with advancements in the field, the cost associated with such devices have fallen drastically. It might be that in 50 years time, this trend will continue to GaN and InGaN devices. As stated in the introduction in this report, fire was used as the major source of lighting for thousands of years. In this context, a time span of 50 years is not long.

## Acknowledgements

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Finally, I would like to thank the Crosslight team for providing licences to their TCAD software which was not only instrumental in this project, but also a great educational tool.

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