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Investigation of Optical Losses in Quantum Dot Color-converting Layers Using Ray-tracing Model

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ABSTRACT

Optical modeling (ray-tracing) of a simplified green QD-OLED pixel is used as a tool to identify and explore the major loss mechanisms within this system. Parameters of the QD layer that are varied in the model to determine the effect on losses include QD loading, thickness/aspect ratio, and the use of scattering agents. Additional changes to pixel material properties such as sidewall reflectivity are modeled to highlight the impact that material improvements can make to the overall device output. This modeling approach and learnings can be applied to any device where color conversion is required, such as QD-OLED and microLEDs.

1 Introduction

Quantum Dots (QDs) have become an enabling technology for new displays due to their ability to efficiently convert blue light to red and green. Their small size, strong absorption, and tunable, narrow emission spectra provide unique advantages over phosphor technology when used in color conversion applications where film thickness is on the order of microns and where printing technology is used to pattern sub-pixels. A promising implementation of QDs as a color converter for displays has come in the form of QD-OLED where a blue AM-OLED source is used to illuminate patterned red and green QD sub-pixels resulting in excellent contrast, color, brightness and viewing angle. It is widely known that QD-OLED panels require the use of an additional color filter (beyond the QD layer) to achieve the desired color metrics due to leakage of blue light through the thin QD layers. In particular, green QDs have been the most challenging material to achieve complete color conversion (lack of blue leakage) due to lower absorption of blue photons compared to other QD colors (especially for InP). When incomplete absorption occurs, some blue photons pass through the QD layer, reducing the color purity. While it is possible to increase the thickness and concentration of the QD layer or implement an additional color filter on top of the red and green sub-pixels, these changes are undesirable from a cost and manufacturing perspective. Optical modeling can be used to investigate how properties of the QD layer will impact display performance. Leveraging new material advancements and optimization via modeling, the color filter could be eliminated if the blue leakage can be reduced while maintaining green output.

It has been speculated that an additional green OLED layer is included in the blue OLED stack to enhance brightness of the display. Employing optical modeling to improve our understanding of the loss mechanisms may help drive improvements to eliminate additional green OLED layers and save cost.

Optical modeling of illumination systems, also referred to as non-sequential modeling, is a software-based method for the analysis of an optical system comprising one or more sources of photons and the geometrical materials with which they interact. The ability to model complex optical systems with a multitude of light paths can be an extremely effective tool for system design and development. In the process of modeling, solid models of all components in an optical system are created with appropriate material and optical interface properties applied. Up to millions of rays with a desired distribution of spatial origin and angular trajectories are placed within the system and the paths of all rays are calculated using Monte Carlo methods based on interactions with the components. Ray receivers are placed at desired locations to intercept rays and gain an understanding of the spatial, angular, and spectral distributions of illumination patterns in these locations (Figure 1). A

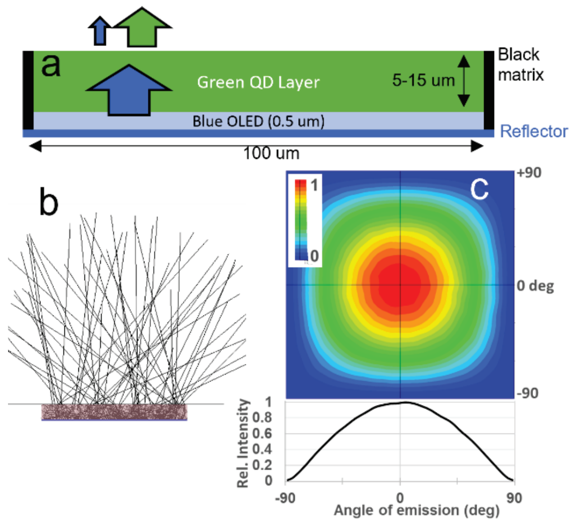

Figure 1. Diagram of green QD-OLED subpixel showing partial conversion of blue photons into green (a, not to scale), sub-set of rays resulting from optical model (b), and heatmap of green photon intensity (angular) pattern with the profile of a central slice through the pattern (c).

major advantage of non-sequential modeling is the ability to predict system performance and explore trends over a wide range of system variables without the time and expense of physical prototyping. Frequent uses are to identify contributors to lower than expected performance, improve quality management by predicting performance variability, drive the development of improved materials, and provide a foundation for engagement with customers. In this study, optical modeling is used to investigate the optical performance of a QD-OLED sub-pixel as a function of various key geometric and material parameters. Of particular interest are the loss mechanisms and how the use of new materials could improve the output of QD-OLED or microLED devices.

2 Methods

Optical modeling of a simplified green QD-OLED sub-pixel was performed using LightTools v9.1.0 illumination design software (Synopsys). Details of the optical model can be found in prior literature[1] and Figure 1. Briefly, an OLED source emitting blue photons is situated below the color converting layer containing green QDs. Optical properties of the OLED were measured from an iPhone12, while the QD optical properties were taken from literature.[2] In some cases scattering particles are also included in the form of TiO_2. The model was set up such that the thickness of the QD layer and optical properties of all components could be easily adjusted to provide data on a wide range of variables. All components were built in LightTools and analyzed using a combination of LightTools internal suite of reporting and analysis tools as well as external software.

Output from the simulations (Figure 1) consists of irradiance and intensity profiles along with the photon wavelength all captured directly just above the surface of the device. Simulations were run with 1W of blue photon power for simple ratiometric evaluation of power emitted from the pixel. One million rays were launched from the blue OLED, and the LightTools ray report tool was used to evaluate the ray paths of all one million rays to determine where rays were lost, for example due to pixel architecture absorption, QD quantum yield loss, or QD Stokes loss. This method allows for thorough investigation of optical losses in the system.

Results derived from modeling will, in general, not match measured devices perfectly due to differences in geometry and material properties. However, even the simple model used here can be very useful for exploration of trends and identifying major loss mechanisms of a new technology to inform design choices.

3 Results and Discussion

To demonstrate the sensitivity of device performance to four key variables, and to demonstrate the capability of modeling to reveal trends in performance with these variables, four groups of simulations were performed as follows:

Table 1. Four groups of simulations

	A	B	C	D
QD (wt%)	**10-30**	30	30	30
QD thick (µm)	10	**5-15**	10	10
Scatter (wt%)	1	1	**0-10**	**1-10**
Wall %R	0	0	0	**0-100**

The primary output captured by the model is the power of green photons and blue photons exiting the device relative to the power emitted from the OLED. Figure 2 captures these trends as a function of QD concentration (Group A simulations, Figure 2a), QD layer thickness (Group B simulations, Figure 2b), and scatterer concentration (Group C simulations, Figure 2c). The maximum green power emitted in any of these cases is about 30% of the original OLED Power. 70% of the blue photon power is lost to a combination of absorption in the device components, blue leakage, and Stokes or QY loss from the color conversion process.

Figure 3 looks at the loss categories in more detail for the group C data set. The conversion loss category (gray) consists of optical losses due to lower than unity PLQY as well as Stokes losses. While we can model variations in PLQY, we chose a reasonable reported value of 95%.[2] The Stokes loss from a blue photon (2.70 eV) to a green photon (2.35 eV) cannot be changed. In all three cases the largest loss category is the black matrix (BM). Any photon that interacts with a wall is absorbed, and while the device has an aspect ratio that is fairly small (10 µm tall, 100 µm wide) it appears there

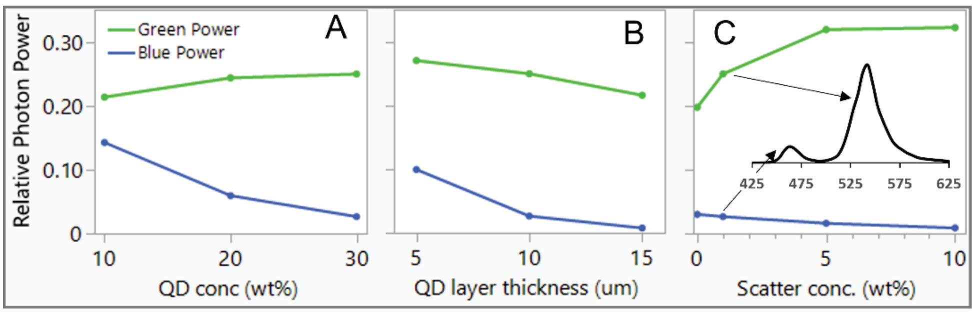

Figure 2. Relative green and blue photon power emitted from the pixel as a function QD concentration (Group A, 1% scatter) QD layer thickness (Group B), and scatterer concentration (Group C). Inset is a representative optical spectrum.

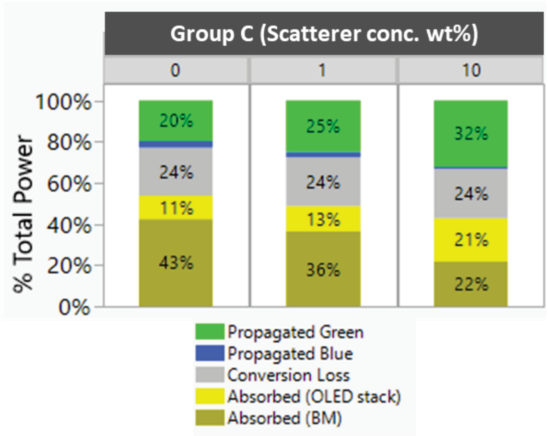

Figure 3. Breakdown of location of optical power losses in the system after blue photon emission from OLED.

is still substantial interaction of photons with the walls of the device.

Group D simulations explore efficiency gains if the walls of the device are not black, but instead partially or fully reflective (0-50-100%R) at two different scatterer loadings (Figure 4). While a 100% reflective case may be unrealistic, it will, at a minimum, provide us with an upper bound to understand how changing the optical properties of the wall could impact device performance. Significant gains in green photon output are observed when %R is increased (Figure 4). The trend with scatter concentration remains intact, with higher scatter leading to increased green output, however the effect is muted with 100%R walls since the #1 loss category is now eliminated.

As expected, optical losses due to absorption by the device walls decreases significantly as the reflectivity of the walls increases. Only a portion of these photons are re-allocated to the desired "propagated green" category. OLED stack absorption increases as the wall reflectivity increases, especially in the 100%R case. Since more photons remain within the QD matrix, there is additional opportunity for green emitted photons to interact with the OLED stack which has a non-zero probability of absorbing these photons.

Interestingly, blue photon leakage (Figure 4) does not change significantly as the wall properties are changed - a desirable result. This indicates that there are not many blue photons interacting with the device walls, or that the blue photons reflected from the walls are then absorbed by QDs or lost due to other mechanisms.

Green power output increases with increased scatter loading regardless of the wall reflectivity (Figure 4). The impact of scatter concentration is more pronounced when the reflectivity is set to 0% or 50%. At low scatter loading we expect higher interaction between photons and the device wall since there is less redirection of photons by scattering centers. When the low scatter loading coincides with high reflectivity of the wall there is significantly less photon loss because more photons interact with the highly reflective wall. This is the main reason that the impact of green output is less dependent on scatter loading when wall reflectivity is increased.

4 Conclusion

Optical modeling of a green QD-OLED sub-pixel has proved to be an effective way to identify major loss mechanisms and explore changes in material properties to improve device performance. Modeling suggests that adjustment of the reflectivity of the device walls has potential to significantly improve the device output without impacting the undesirable leakage of blue photons. It is possible that this adjustment could impact other important parameters such as reflection handing in high ambient light situations.

While the modeling was performed on QD-OLED, the same approach can be considered for other advanced display technologies such as microLED which will face similar challenges to QD-OLED. These findings suggest that new material options should be explored for use with new display technologies such as QD-OLED and microLEDs that incorporate color conversion.

References

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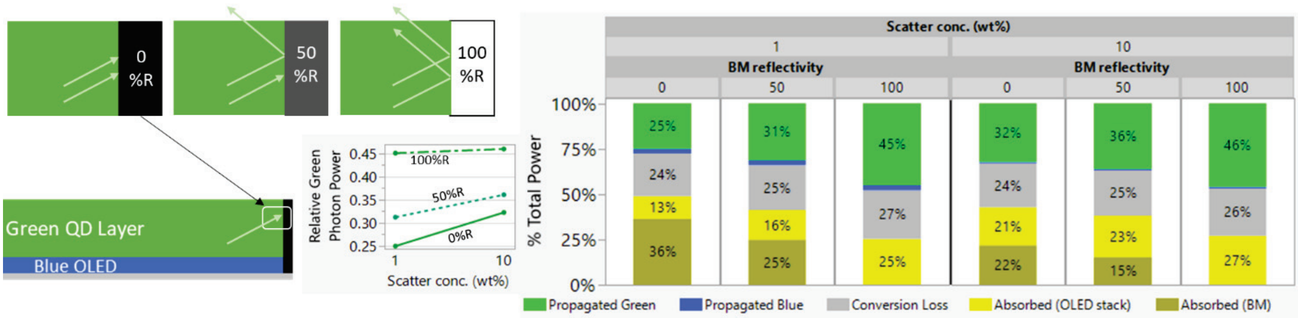

Figure 4. Diagrams of 0-50-100%R cases (group D) along with green power output for each case as a function of scatter loading. Bar chart shows location of optical power losses in the system.