

# Simulations, Measurements and Optimization of OLEDs with Scatter Layer

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## Abstract

*A multi-scale optical model for organic light-emitting devices containing scattering layers is presented. This model describes the radiation of embedded oscillating dipoles and scattering from spherical particles. After successful model validation with experiments on a top-emitting white OLED, we show how this tool can be used for optimization with specific targets.*

## Author Keywords

OLED; simulation; light-scattering; Mie particles; color point.

## 1. Introduction

Improved light out-coupling is at the heart of the future development and commercialization of organic light emitting diodes (OLEDs) for (general) lighting applications as it impacts directly the achievable luminous emission ( $\text{lm}/\text{m}^2$ ), luminous efficacy ( $\text{lm}/\text{W}$ ) and lifetime [1]. State of the art OLEDs emitting white light (WOLEDs) have reached the luminous efficacy of fluorescent lamps ( $60\text{-}100 \text{ lm}/\text{W}$ ) at brightness levels of  $1000 \text{ cd}/\text{m}^2$  and more, they have the potential to reach and overcome the  $100 \text{ lm}/\text{W}$  barrier. It is clear that this goal can only be achieved by improved light out-coupling (ILO), as the best WOLEDs demonstrated to date with ILO are more than two times more efficient than the best ones without ILO. Furthermore one should keep in mind that besides lumens per watt, the targeted emitted color [2] is of equal importance.

The improvement of light out-coupling requires having simulation tools at hand to efficiently simulate such OLEDs that include light out-coupling enhancement structures. The approach that we have developed [3] is to couple the nano-optical properties of the light emission coming from the recombination of electrons and holes with geometrical optics laws to describe light out-coupling structures. This approach has the advantage to be computationally very efficient and lends itself to optimization of device parameters.

In this contribution, we aim to demonstrate the usefulness of such modelling approach by comparing experimental characterizations with simulations of OLEDs embedding a scattering layer made of spherical particles as external out-coupling structure. This out-coupling approach, using particle scattering, was experimentally shown to be very efficient [4, 5].

However, in order to optimize the overall extraction efficiency, it is necessary to tune the thin film OLED stack and the scattering parameters simultaneously using a physically accurate model [3] unlike the simplified modeling approaches used in [4, 5].

In order to run simulations of OLEDs including particle scattering foils, we developed and added a Mie scattering solver to the multi-scale electro-optical OLED simulator of the commercial software SETFOS and is now available in the new version 4.1 [6]. This allows fast simulations of the full OLED structure containing

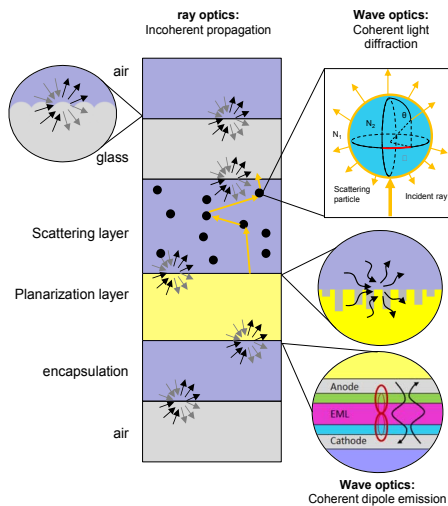
the out-coupling foil. Using this innovative tool a successful comparison between experiments, of a top-emitting OLED with scatter foils, and corresponding simulations is performed and presented in this paper. This model validation proves that such simulations can be used for optimization of OLEDs with arbitrary combination of scattering structures such as nano- and micro-textures (not shown in this contribution), and particle scattering films. At the end, such a device optimization by simulations is carried out, for the case of OLEDs containing particles, to provide guidance for further improvement of this particular OLED device.

## 2. Modelling approach

### 2.1. Method description

We have developed an original approach based on a net radiation algorithm [7] to compute the impact of incoherent and scattering layers embedded in the full OLED stack. This approach relies on the same physical assumptions as a traditional one involving a ray-tracing tool [8]: while the wave nature of light is considered in the thin film layer stack that contains the emitting dipoles, only the intensity of light is considered in thick incoherent layers (see Figure 1). However, the mathematical way to solve the problem does not rely on a Monte-Carlo algorithm, which is the case in ray-tracing simulations. As described in Figure 1, we first compute the light emission coming from the emissive dipoles [9] in the two incoherent layers surrounding the thin films stack embedding the emitting dipoles. Then, light propagation through the layers and multiple reflection and transmission at the interfaces connect the light fluxes in the different layers. For a specific test OLED structure, we previously successfully benchmarked this innovative modelling approach with the traditional approach based on a combination of a dipole emission model for the thin film stack and a ray-tracing tool [3].

In this innovative approach, the transmittance, reflectance and absorption of the scattering layer (bidirectional scattering distribution function, BSDF) are computed for all wavelengths and incident angles using the internal Mie-solver of SETFOS 4.1. The BSDF are then used by the net radiation algorithm introduced above to compute the light emission of the full stack.



**Figure 1.** Schematic representation of the scalar scattering modeling approach for OLED light-out-coupling.

## 2.2. Mie scattering model and validation

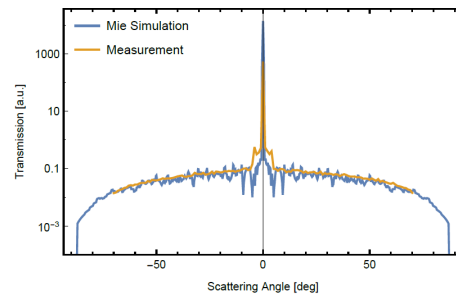
The Mie scattering feature of SETFOS is used to compute the BSDF of layers containing scattering spherical particles. This feature allows the user to consider only one type of particles (mono-disperse) or different type of particles (poly-disperse). The scattering properties, including the cross section and the far-field scattering distribution of each individual type of particles which both depend on the optical indexes and the size of the particle, are computed using the Mie theory [10], which relies on wave-optical physics. A ray-tracing algorithm (relying on ray-optics assumption) is used to account for the light propagation between each scattering event assuming randomly distributed particles in the layer.

In order to validate the Mie particle layer scattering model we have compared the simulated transmittance of a reference layer stack with the measurement. The stack consists of a glass coated with a high index layer ( $n=1.7$ ) containing Mie particles. On top of it, a thin ITO layer was deposited. The scattering layer has the following characteristics:

- The matrix layer embedding the Mie particles has a thickness of 4 micrometers
- $\text{SiO}_2$  particles ( $n=1.45$ ) with a diameter = 330nm serve as scattering particles.
- The particle concentration is 5%

The transmittance measurement was performed at a wavelength of 545 nm with an illumination from the ITO side.

The measured and simulated transmittance is shown in Figure 2. A very good agreement was found. In the measurement, the small transmission intensity shoulder for  $\pm 5$  degrees observation angle is an artefact due to the laser beam shape. This difference between experiments and simulations can be disregarded.



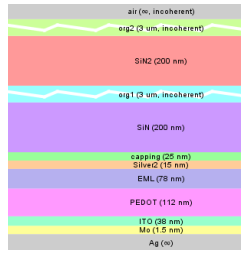
**Figure 2.** Comparison between measured and simulated angular transmission of a scattering layer. The simulation uses the Mie scattering algorithm of SETFOS 4.1 [4].

## 3. Model validation with experiments

In the previous section, a successful benchmark between measurement and simulation of the transmittance of a scattering layer was shown. In this section we aim to use this model to simulate and experimentally validate our complete simulation workflow spanning from the dipole emission to the full OLED stack, including thick encapsulation layers and scattering layers. A  $2 \times 2 \text{ cm}^2$  OLED was fabricated on a glass substrate onto which a 100 nm thick silver reflector was evaporated. An ITO layer of 40 nm was deposited by RF-sputtering, followed by spin-coating of a  $\sim 110 \text{ nm}$  PEDOT:PSS layer (Orgacon by Agfa Gevaert, Be). Next, 80 nm of a fluorescent white light-emitting polymer (Merck KGaA, De) was spin-coated from toluene solution. The semi-transparent cathode stack, consisting of Ba, Al, Ag and ZnS, was deposited by thermal evaporation. This cathode stack has a transparency of about 60-70%. A thin film encapsulation stack, developed by the Holst Centre, was then deposited. The stack consists of an optically thick organic layer sandwiched between two inorganic high index layers (SiN). In Figure 3 the OLED device structure is sketched. Finally, a top coat was applied onto the thin film encapsulation. Scattering of light emitted by the OLED was accomplished by bringing a 100 micron thick hazy PET foil (DuPont Teijin Films, UK) in optical contact using an index matching oil ( $n=1.574$ , Cargille Labs, USA). This PET foil can be removed and exchanged by another PET foil, allowing us to evaluate the impact of scattering using the same OLED stack. Three different white OLED devices were investigated:

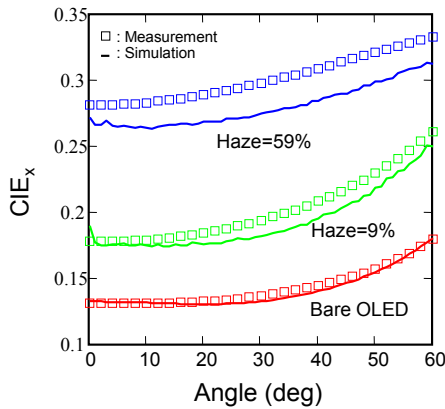
- Without scattering foil
- Using a scattering foil with a haze of 9%
- With a scatter foil with a haze of 59%

The scatter foil resulting in a haze equal to 59% showed absorption of approximately 1.6%. In order to capture this effect, a small imaginary part of approximately  $k=10^{-3}$  was added to the optical index of the particles. The particle concentration was tuned so as to get the same haze as the measured scattering foils. Note that the structure of Figure 3 shows a combination of optically thick and thin film layers.

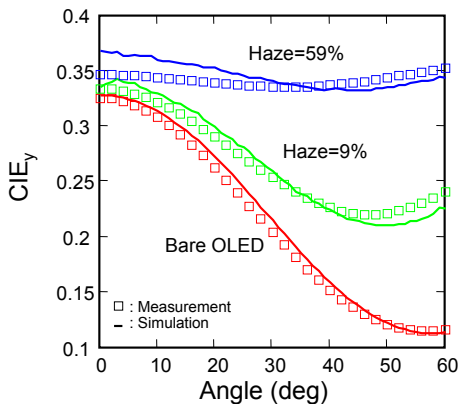


**Figure 3.** Schematic of the OLED device stack with thin film encapsulation on top of which two distinct scattering foils were applied.

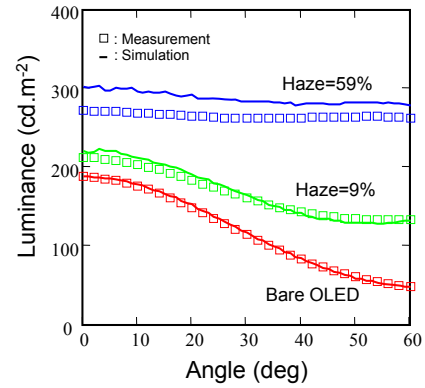
Our optical simulations could nicely reproduce the measurements of the reference case, the case of using a 9% haze foil and the case of a 59% haze foil on top of the OLED. It can be noted in Figure 4 and 5 that the emitted color of the OLED drastically changed from blue (bare OLED) to almost white ( $CIE_x$  is almost 0.3) when applying the 59% haze scattering foil. This reveals that red and green wavelengths were strongly wave-guided in the reference device stack. Obviously, applying a scattering foil on the device helped to couple out these colors.



**Figure 4.** Simulation (lines) and measurement (squared dots) of the  $CIE_x$  point of the bare OLED (red), OLED + 9% haze scattering foil (green) and OLED + 59% haze scattering foil (blue).



**Figure 5.** Simulation (lines) and measurement (squared dots) of the  $CIE_y$  point of the bare OLED (red), OLED + 9% haze scattering foil (green) and OLED + 59% haze scattering foil (blue).



**Figure 6.** Simulation (lines) and measurement (squared dots) of the luminance versus the observation angle of the bare OLED (red), OLED + 9% haze scattering foil (green) and OLED + 59% haze scattering foil (blue).

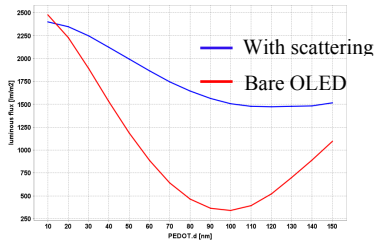
As shown in Figure 6, the luminance of the OLED is strongly increased when making use of a scattering PET foil (leading to an integrated radiance increase of approximately 220%). We note that the enhancement is stronger for larger viewing angles. This can be understood considering the fact that for light incident to the particle scattering layer at oblique angles, the number of scattering events is higher than for normal incidence. It is notable, that the angular luminance achieved with applying the 59% haze foil is almost independent of the viewing angle.

#### 4. Device optimization

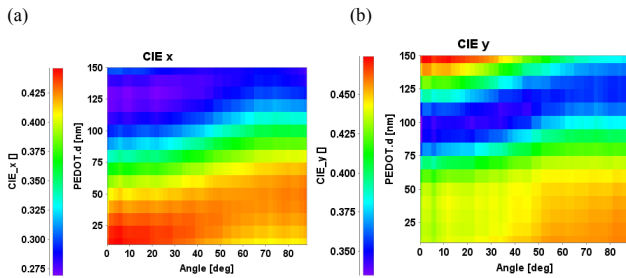
In the previous section, we have shown that the simulations using SETFOS 4.1 could nicely reproduce experimental characterizations of white OLEDs containing scattering layers. Our modeling approach allows one to simultaneously vary parameters of the OLED stack and parameters of the scattering layer. Therefore, in this section we will present how the device could be further optimized.

In Figure 7 we show the calculated luminous flux obtained using a bare OLED and a scattering foil (haze = 80%) versus the thickness of the PEDOT layer. We can observe that for extremely thin thicknesses, the emitted luminous flux of the bare OLED can be similar to the one prepared with a scattering foil. However extremely thin layers of PEDOT might not be relevant for deposition reasons.

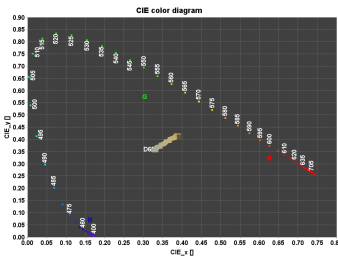
Also, one can be interested into achieving an emitted color close to a warm white. Simulations, not shown here, have revealed that using an OLED like in Figure 3 without scattering layer, it was impossible to achieve a white emitted color by varying the thickness of the PEDOT:PSS layer. However, using an 80% hazy foil and varying the thickness of the PEDOT layer, it seems possible to achieve a white emitted color ( $CIE_{x,y} \approx 0.33$ ) (Figure 8), for a thickness around 90 nm. After optimization, an optimal thickness of the PEDOT layer of 85 nm was found, the CIE point of the device versus the angle is shown in the CIE diagram in Figure 9. This figure shows that indeed a warm white OLED can be obtained.



**Figure 7.** Simulation of the luminous flux of the OLED detailed in Figure 3 versus the thickness of the PEDOT layer.

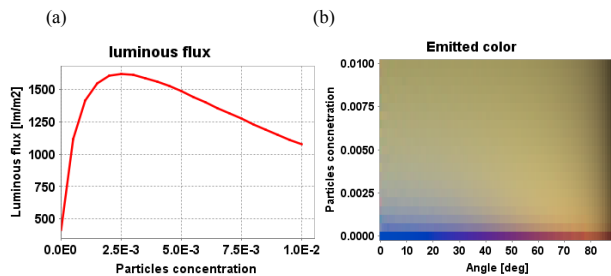


**Figure 8.** Simulation the color point coordinate (a) CIE<sub>x</sub> and (b) CIE<sub>y</sub> versus the thickness of the PEDOT layer.



**Figure 9.** Simulation the color point coordinate versus the angle for a 80% hazy foil and a 85 nm thick PEDOT:PSS layer.

Finally, as presented in Figure 10, it is also interesting to see how the luminous flux and color emitted by the OLED would change by varying the concentration of scattering particles (and thus the haze) embedded in the PET foil. We can find an optimum for the luminance for a concentration of 0.25% leading to a haze of 67%. For higher concentration the out-coupling efficiency tends to decrease because of the absorption of particles and a bigger reflectance of the scattering foil. We can also notice that the emitted color tends to be more and more stable versus the angle when the concentration of particles and the haze are increased.



**Figure 10.** Simulation of the luminous flux (a) and emitted color versus the concentration of scattering particles in the PET foil for viewing angles between 0 and 90 degrees (b).

## 5. Conclusion

After presenting the modelling procedure implemented in SETFOS 4.1 for the simulation of OLEDs containing a scattering layer, we have shown that this powerful tool reproduces experimental measurements of a top-emitting white OLED both in terms of luminance and color. The validation was carried out with angular measurements up to a viewing angle of 60 degrees. Finally we have demonstrated how to use this optical simulation method for optimizing the device with specific targets concerning both the emitted color and the efficiency of the device. Since this optical emission model is seamlessly integrated with the charge drift-diffusion module of the software SETFOS [6], a comprehensive simulator is available for OLED characterization and optimization.

## 6. Acknowledgements

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