Optimization of OLED performance by optical modeling

R. Nitsche[1], M. Furno[2], R. Meerheim[2], B. Lüssem[2] and K. Leo[2]
[1]sim4tec GmbH, Dresden, Germany
Tel.: +49 351 4466499, E-mail: info@sim4tec.com
[2]Technische Universität Dresden, Institut für Angewandte Physik / Photophysik, Dresden, Germany

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Abstract

In this paper we demonstrate how to use optical simulation to enhance OLED performance. Using state-of-the-art p-i-n OLEDs, we validate our optical model by fitting key figures like current, power, and quantum efficiencies to the experimental results. We finally provide general design guidelines for optically optimized OLEDs.

1. Introduction

The development of highly efficient multilayer OLEDs has so far mainly been achieved by experimental trial and error methods and is therefore cost intensive and time consuming. A potentially much cheaper and faster approach is to conduct numerical simulations for device design and optimization beforehand, thus reducing the experimental work significantly and gaining a deep understanding of OLED device physics.

In this contribution, we demonstrate an optical optimization study of a p-i-n bottom emitting red phosphorescent OLED [1] by means of numerical simulations using the integral OLED device simulator SimOLED®. Our goal is to find an optimal device configuration with respect to the key figures current efficiency (CE), power efficiency (PE), and quantum efficiency (QE), by varying the thickness of the hole transport layer of the OLED.

2. The device simulator SimOLED® / Experimental Setup

The device simulator SimOLED® is able to calculate both, electrical (e.g. current-voltage), and optical (e.g. spectral luminance vs. voltage) characteristics of OLEDs. We have already presented general models and results about the electrical and optical part of SimOLED® in a different publication [2] so we will not repeat this here. Here, we extend the optical modeling to include the calculation of CE, PE, QE and CIE color coordinates (no results shown in this contribution). Additionally, the software can now perform fast automatic parameter variations which enable the use of automatic optimization and fitting routines.

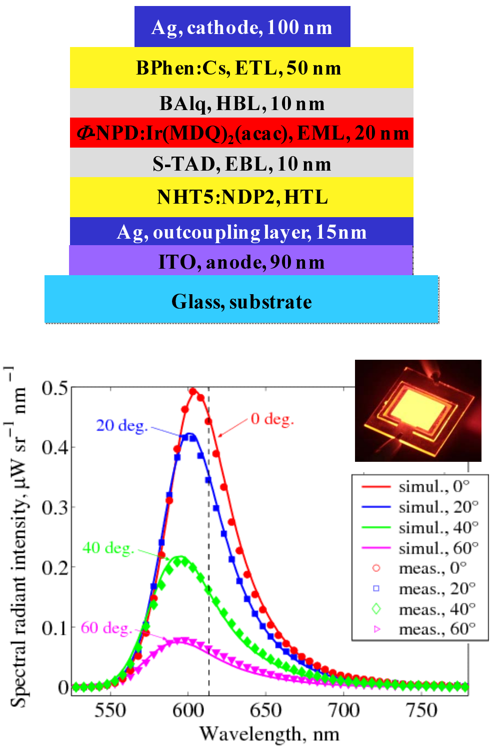

Fig. 1. OLED setup (top), and comparison between simulated (solid lines) and experimental (symbols) data (bottom).

The OLED to be optimized is shown in Figure 1 (top panel). It corresponds to a classical bottom emission OLED with an additional thin Ag layer in between ITO and NHT5:NDP2, which serves as outcoupling enhancement layer [3]. The thickness of the doped HTL is to be varied in the simulations to achieve an optimal device design. This will not affect the electrical properties of the OLED since there is virtually no voltage drop over this layer due to the effective electrical doping.

3. Results and discussion

The spectrally and angularly resolved OLED emission as well as CE, PE and QE have been simulated and measured as a function of HTL thickness. Figure 1 (bottom panel) shows a typical comparison between measured and calculated spectral results, with a very good overall agreement. In order to achieve such a fit only slight variations of the layer thicknesses on the order of 5-10 % (well within the experimental error) had to be applied. We use a single dipole placed at the interface between the EML and the EBL as the light generating source. The specific location of that dipole is motivated by our own electrical simulations (not shown here) as well as by the fact that holes can enter the EML much easier than electrons, causing a peaked recombination profile at the interface between EML and EBL. For a single dipole located at the interface between the EML and HBL the quality of fit is strongly reduced, confirming the assumption made above. The data of Figure 1 (bottom panel) have also been used to calibrate our optical model to the experimental data to get absolute quantities from the optical simulation. We stress that only one global calibration factor had to be used for all simulation results presented here.

To find the optimal device configuration we varied the HTL thickness d_{opt} and calculated CE, PE and QE (plotted in Figure 2). The overall agreement to the experimental data is again very good, confirming the underlying physical models [2]. We can nicely predict the optimal HTL thicknesses for each OLED key figure. For CE we read d_{opt}=45 nm, for PE d_{opt}=50 nm and for QE d_{opt}=60 nm. Apparently, there is no global d_{opt} which maximizes all three key figures at once. The physical root cause is due to the coupling (or the spectral overlap) between the emitter spectrum and the white light spectrum of the OLED cavity. The white light spectrum is defined as the emission intensity outside the OLED which is caused by an emitter (inside the OLED) radiating with an intensity of 1 for all wavelengths considered. It is thus a quantity independent of the specific choice of the emitter, characterizing the optical properties of the (passive) OLED microcavity only. By varying the HTL thickness the spectral and angular dependency of the white light spectrum strongly changes and so does the coupling to the emitter spectrum, prohibiting the occurrence of a global d_{opt}.

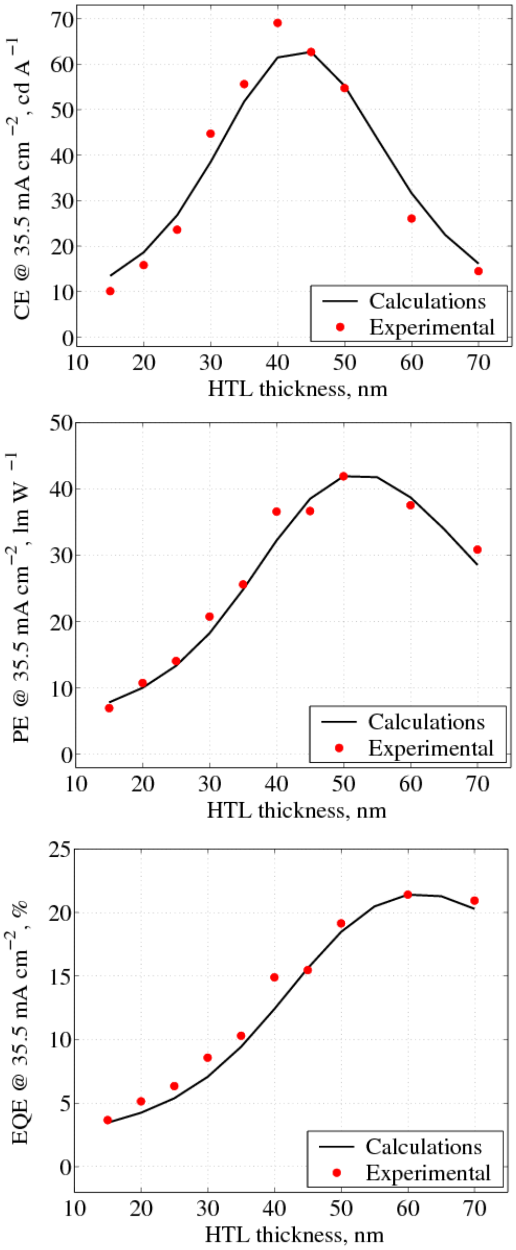

Fig. 2. Simulated (solid lines) and experimental (symbols) data of CE (top), PE (middle) and QE (bottom) as a function of HTL thickness.

To demonstrate that issue in greater detail we have investigated the case of a completely detuned OLED employing a HTL thickness of 70 nm. The measured and calculated emission spectra as well as the calculated white light spectra are shown in Figure 3. Again, the agreement between simulated and measured data is very good, confirming our previously found parameter set. The effect of the detuned OLED microcavity is nicely seen through a strong red-shift of the emitter peak from ~620 nm (dashed line, plain emitter material, no microcavity) to ~670 nm for an observation angle of 0° (representative for CE). The reason is that white light spectrum and emitter spectrum do not overlap very well for 0° or in other words, the emitter dipoles couple rather poorly to the OLED microcavity, yielding a very low CE. The best coupling is achieved for the afore mentioned d_{opt} = 45 nm.

The same arguments also hold for the explanation of the optimal thicknesses for PE and QE. However, in these cases we also have to look at observation angles off normal since they also contribute to PE and QE. Figure 4 shows the white light spectra of the optimal HTL thicknesses for CE (top panel) and QE (bottom panel). Due to the strong blue shift of the spectra with increasing observation angle one observes a poor coupling of the emitter to the microcavity for the CE case at larger angles, leading to a low value of the QE. On the other hand, for the optimal thickness for QE the coupling to the emitter at larger angles is much more effective than before at the expense of a lower coupling at 0°. Despite the latter, *on (angular) average* this configuration yields an improved QE, since more photons are outcoupled.

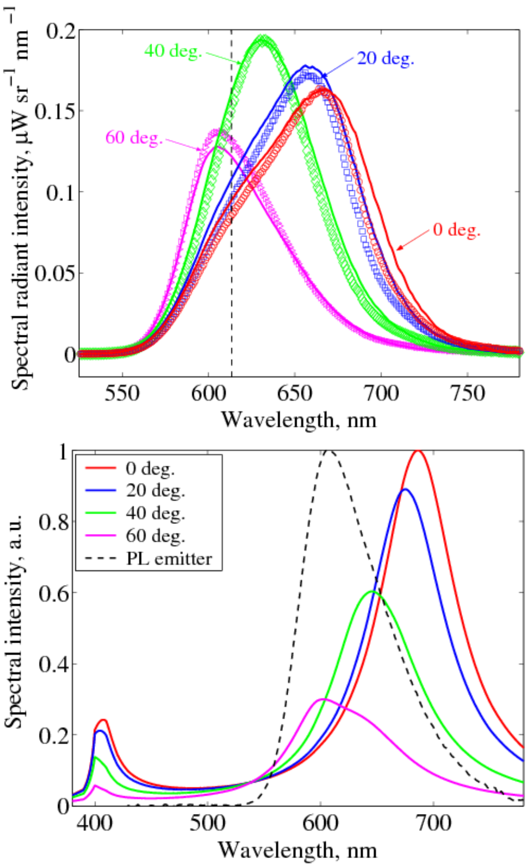

Fig. 3. Simulated (solid lines) and measured (symbols) emission spectra (top) and simulated white light spectra (bottom) of the OLED of Fig. 1 with an HTL thickness of 70 nm. The dashed grey spectrum corresponds to the PL spectrum of the plain emitter.

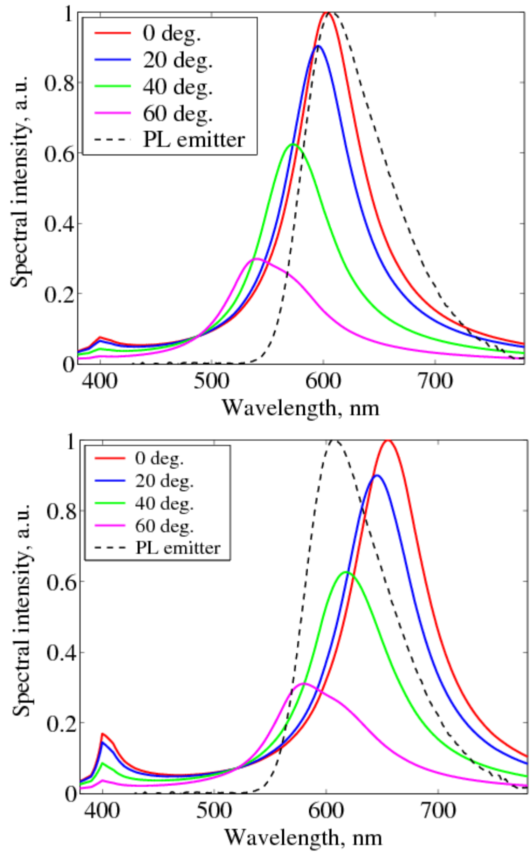

Fig. 4. Simulated white light spectra for the optimal CE case (top) and optimal QE case (bottom). The dashed grey spectrum corresponds to the PL spectrum of the plain emitter.

From these considerations it becomes clear that a simultaneous optimization of CE, PE and QE is not possible for the OLED investigated here. However, depending on the target application (e.g. maximal forward emission vs. maximal outcoupled total power), SimOLED® can be used to design the desired OLED with minimal efforts.

4. General Design Guidelines

In order to optically optimize an OLED one first has to find a suitable experimental calibration set, since the optical simulation will only give relative quantities. By using such an experimental set, the simulated data are calibrated by a *global* scaling factor to yield absolute values which can directly be compared to other optical measurements of the same OLED. During this calibration process the thicknesses of the individual layers may have to be slightly adjusted to account for experimental errors.

Secondly, some information about the exciton (or dipole) profile within the emitting layer(s) has to be provided. This can be gained by qualitative considerations of mobilities and energy levels of the materials adjacent to the EML or by using the electrical simulation capabilities of SimOLED®. For most cases, a single dipole placed at a certain location within the EML might already be sufficient, unless the EML happens to be rather thick as it might be the case for some polymer OLEDs.

Third, one has to choose the quantity to be optimized, since usually not all key figures can be optimized simultaneously, as has been shown above. Considerations concerning color stability (reflected in the dependence of the CIE coordinates as a function of e.g. observation angle) may also be taken into account at that point.

Finally, the device can be optimized automatically in SimOLED® by scanning appropriate parameters like layer thicknesses or refractive indices within a certain parameter range. Care has to be taken as not to change the electrical properties of the device at the same time since this alters the exciton distribution and therefore the outcoupling of light as well. The differentiation between optical and electrical optimization is than not possible anymore. Good candidates for (optical) layer thickness optimizations are materials that are well conducting like metals (as electrode materials) and doped transport layers or materials that are placed outside the electrically active region like capping layers deposited on top of the (semi-transparent) top contact of a top emitting OLED.

5. Summary

In conclusion, we have used our optical simulation tool SimOLED® to predict optimal device configurations for a red p-i-n OLED aiming at maximum CE, PE and QE, respectively, in very good agreement with the experiment. We could not find a configuration in which all three quantities are maximized simultaneously. The root cause is the coupling of the emitter to the cavity spectrum which can be nicely demonstrated with our optical simulation tool SimOLED®. General design guidelines have been provided by which a desired optimization task can be carried out efficiently using an optical simulation software like SimOLED®. We therefore believe that optical simulation is an effective tool for the optical design of OLEDs since it significantly reduces expensive and time consuming experiments and greatly enhances the understanding of the underlying physics.

Acknowledgement

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6. References

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