A Novel Approach for OLED Simulations

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Abstract—In this work, we present a comprehensive and experimentally validated model suitable for the quantitative description of all relevant physical processes determining the efficiency of organic light emitting diodes (OLEDs). The modelling approach includes a numerical electromagnetic model developed to quantify the outcoupling efficiency of planar OLED structures. The optical model, coupled with an approximate formulation for the excitonic and electrical processes taking place in OLED devices under electrical operation, provides a quantitative description for the key optoelectronic figures-of-merit of OLEDs. The application of the proposed model to state-of-the-art OLED devices allows for a clear identification of all efficiency loss channels in the devices under study.

I. INTRODUCTION

During the last decades, organic light emitting diodes (OLEDs) have experienced a tremendous increase in efficiency and stability [1]. To overcome the efficiency limitations of state-of-the-art OLED devices, a physically thorough understanding of the most relevant processes at the basis of OLED operation is mandatory.

Due to the number and complexity of the different physical mechanisms involved with OLED operation and to the lack of a unified theoretical description for such processes, a certain degree of approximation has to be introduced in any current OLED modelling strategy. Although OLED optical modelling can be considered as a field with a substantial maturity [2], [3], [4], [5], [6], the current understanding of electrical (and partially excitonic) processes in OLEDs is still far from being satisfactory and therefore none of the existing models is applicable to real-world devices.

The aim of this work is to fill the gap between the available modelling techniques and experiment. To this purpose, we propose a simplified description for charge and exciton dynamics in OLEDs, for which no accurate models and modelling parameters are available at present. Such an approximate description is coupled with a rigorous description for OLED optics.

II. THE OLED MODEL

A. Modelling of Electrical and Excitonic Processes

Electrical and excitonic processes contribute the determination of the number of radiative events per unit time and unit area occurring in an OLED device for a given amount of electrical charges injected into the device. The exciton concentration s in the OLED active layer is given by the solution of the exciton rate equation [7] at all positions z within the EML. We assume exciton annihilation processes to be negligible if the OLED is operated at low current densities.

By further assuming a position-independent exciton generation profile G, it can be demonstrated [8] that the number of decaying excitons per unit time and unit area S is obtained as $S = Gd$, where d denotes the thickness of the EML. The exciton generation term G would ideally be the result of an electrical simulation, but the currently available OLED electrical models does not allow to quantitatively estimate such a quantity. Therefore, we consider the concentration S as a *first* fitting parameter to be extracted from the experiment.

The second modelling step consists of the calculation of the number of radiative excitonic decay events. The intrinsic radiative efficiency of the emitting material being $\eta_{\mathrm{rad},0}$, it can be demonstrated that the radiative emitter efficiency η_{rad} in a microcavity is [9]

$$\eta_{\mathrm{rad}}(\lambda) = \eta_{\mathrm{rad},0}F(\lambda)/\left(\eta_{\mathrm{rad},0}F(\lambda) + 1 - \eta_{\mathrm{rad},0}\right), \quad (1)$$

where $F(\lambda)$ is the wavelength-dependent total power radiated by the emitter. The intrinsic radiative efficiency of the emitter $\eta_{\mathrm{rad},0}$ is the *second* fitting parameter to be extracted from the experiment.

B. The Optical Model

Radiative excitonic decay is treated classically and modelled as forced damped dipole oscillators radiating electromagnetic power [10]. This treatment allows for the calculation of the wavelength-dependent total radiated power $F(\lambda)$ at the location of the emitting dipoles, once the value of the electrical component of the total EM field is known. A transfer matrix approach is exploited for the evaluation of the optical field in planar OLED structures according to the description in [2]. By application of the EM model, the outcoupled fraction $U(\lambda)$ of the total power $F(\lambda)$ is also calculated (see [2], [9] for details). Finally, the spectrally resolved outcoupling efficiency is obtained as $\eta_{\mathrm{out}}(\lambda) = U(\lambda)/F(\lambda)$.

C. Modelling of OLED Efficiencies

The external quantum efficiency of the OLED η_{q} is modelled as the product of the efficiencies of the processes described in the previous subsections. To properly account for the polychromatic nature of the emitting materials used in OLED devices, a normalized spectral distribution $s_{\mathrm{ph}}(\lambda)$ of the emitted photons is included in the model. The EQE is finally given by

$$\eta_{\mathrm{q}} = \frac{eS}{J}\int_{\lambda} s_{\mathrm{ph}}(\lambda)\eta_{\mathrm{rad}}(\lambda)\eta_{\mathrm{out}}(\lambda)\,\mathrm{d}\lambda. \quad (2)$$

Equation (2) is the central theoretical result of this work. It allows for a quantitative numerical description of the EQE of

a given OLED structure by making use of a *limited number of fitting parameters*. Expressions similar to Eq. (2) can be derived for any of the optically measurable characteristics of an OLED, e.g. the luminous efficacy or the luminance in a given direction.

III. RESULTS AND DISCUSSION

The model described in Sec. II has been used to design a set of 16 small-molecule bottom emitting OLEDs based on the *p-i-n* architecture [11], [12] and featuring the phosphorescent emitter $Ir(MDQ)_2(acac)$. The devices are fabricated in one single experimental run by thermal evaporation onto an ITO-covered glass substrate in an UHV chamber (Kurt J. Lesker Company). By employing the OLED optical model, the thickness of the organic layers is optimized to achieve the best performance in terms of external quantum efficiency. The thickness of the electron transport layer (ETL) is varied continuously between 45 and 260 nm.

The measured EQE values on the fabricated devices are shown in Fig. 1. Remarkable are the efficiency values, among the highest ones reported for this class of devices. A four-parameter fitting algorithm is used to extract the relevant modelling parameters from the measured data, namely the OLED electrical efficiency γ, the intrinsic radiative efficiency of the red phosphorescent emitter $\eta_{rad,0}$ and two additional parameters accounting for eventual processing errors. The extracted parameters are $\gamma = 0.95$, $\eta_{rad,0} = 0.85$, and an error on the thickness of the ETL layer equal to 5.5 nm.

Calculation results obtained according to Eq. (2) are compared to experimental results in Fig. 1. The agreement between calculations and measurements is fully satisfactory, indicating that all relevant physical processes are correctly included in the proposed OLED model. The modelling approach allows not only for an effective design and optimization of the OLED structures, but also for a meaningful quantification of the efficiency of all optical, excitonic, and electrical processes [13]. As an example, we estimate for the most efficient device in Fig. 1 ($d_{ETL} = 250$ nm) that electrical and excitonic losses are 19 % of the number of injected electrical charges. Substrate and waveguiding losses are 15 % and 34 %, respectively. Coupling of radiation to surface plasmon polaritons and internal absorption are 5 % and 6 %, respectively. Finally, outcoupled photons account for the 21 % of the injected charge carriers.

IV. CONCLUSION

We have a presented a novel modelling approach suitable for the quantitative simulation of the optoelectronic efficiency of planar OLED devices. The model, applied to a series of small-molecule bottom emitting OLEDs, yields a fully satisfactory agreement with the measured data and can provide useful information about the channels of efficiency loss in the devices under study. We consider the presented modelling approach a powerful tool for the design, optimization and, more in general, the development of the OLED technology.
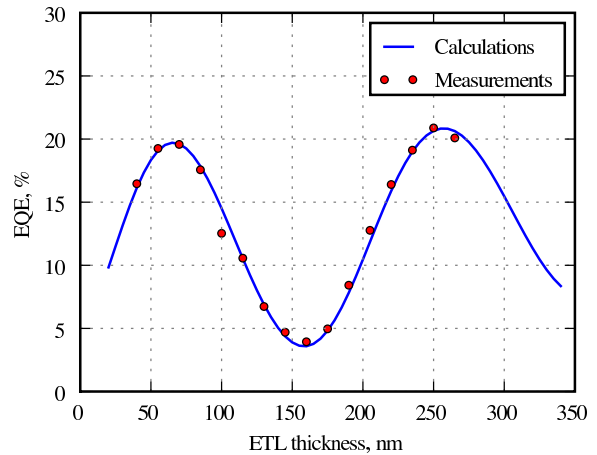

Fig. 1. External quantum efficiency of bottom-emitting red OLEDs. Comparison of simulations and measured data at 1.5 mA cm^{-2} forward current.

REFERENCES

[1] S. Reineke, F. Lindner, G. Schwartz, N. Seidler, K. Walzer, B. Lüssem, and K. Leo, "White organic light-emitting diodes with fluorescent tube efficiency," *Nature*, vol. 459, pp. 234–238, 2009.
[2] M. Furno, R. Meerheim, M. Thomschke, S. Hofmann, B. Lüssem, and K. Leo, "Outcoupling efficiency in small-molecule oleds: from theory to experiment," *Proc. SPIE*, vol. 7617, p. 761716, 2010.
[3] S. Nowy, B. C. Krummacher, J. Frischeisen, N. A. Reinke, and W. Brütting, "Light extraction and optical loss mechanisms in organic light-emitting diodes: Influence of the emitter quantum efficiency," *J. Appl. Phys.*, vol. 104, no. 12, p. 123109, 2008.
[4] S. Mladenovski, K. Neyts, D. Pavicic, A. Werner, and C. Rothe, "Exceptionally efficient organic light emitting devices using high refractive index substrates," *Opt. Express*, vol. 17, pp. 7562–7570, 2009.
[5] M. Flämmich, M. C. Gather, N. Danz, D. Michaelis, and K. Meerholz, "In situ measurement of the internal luminescence quantum efficiency in organic light-emitting diodes," *Appl. Phys. Lett.*, vol. 95, no. 26, p. 263306, 2009.
[6] S. L. M. van Mensfoort, M. Carvelli, M. Megens, D. Wehenkel, M. Bartyzel, H. Greiner, R. A. J. Janssen, and R. Coehoorn, "Measuring the light emission profile in organic light-emitting diodes with nanometre spatial resolution," *Nat. Photonics*, vol. 4, pp. 329–335, 2010.
[7] S. Reineke, K. Walzer, and K. Leo, "Triplet-exciton quenching in organic phosphorescent light-emitting diodes with Ir-based emitters," *Phys. Rev. B*, vol. 75, no. 12, p. 125328, 2007.
[8] M. Furno, R. Meerheim, B. Lüssem, and K. Leo, *in preparation*.
[9] K. A. Neyts, "Simulation of light emission from thin-film microcavities," *J. Opt. Soc. Am. A*, vol. 15, pp. 962–971, 1998.
[10] W. L. Barnes, "Fluorescence near interfaces: the role of photonic mode density," *J. Mod. Optic.*, vol. 45, pp. 661–699, 1998.
[11] K. Walzer, B. Maennig, M. Pfeiffer, and K. Leo, "Highly efficient organic devices based on electrically doped transport layers," *Chem. Rev.*, vol. 107, pp. 1233–1271, 2007.
[12] R. Meerheim, S. Scholz, S. Olthof, G. Schwartz, S. Reineke, K. Walzer, and K. Leo, "Influence of charge balance and exciton distribution on efficiency and lifetime of phosphorescent organic light-emitting devices," *J. Appl. Phys.*, vol. 104, p. 014510, 2008.
[13] R. Meerheim, M. Furno, S. Hofmann, B. Lüssem, and K. Leo, *in preparation*.