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Digital Twins for OLED Lifetime Predictions

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Abstract

R&D of OLEDs devices can benefit from the support of simulations. The highest level of insight can be obtained with 3D kinetic Monte Carlo. Concrete R&D case studies showing how 3D kinetic Monte Carlo simulations can be used to address OLED R&D challenges will be presented.

Author Keywords

OLEDs; simulations; device; organic electronics; efficiency

1 Introduction about OLED R&D challenges

At present, the development of organic electronic devices largely occurs by following empirical recipes and by trial-and-error. This is a cumbersome process that often does not lead to the expected results and unpredictably delays the release of a new product or a new device technology. Rational design, based on predictive device simulations, is currently gaining more and more interest due to the large acceleration it can bring to research and development cycles, thus reducing time-to-market.

Among the top priorities in the OLED industry is to understand, predict and optimize the lifetime of devices. This is a hard challenge due to the multiple pathways in which the device can degrade, especially at the material level. In fact, degradation of few key molecular sites can result in a large and unexpected performance drop. Although experimental characterization of the degradation products is possible, it is usually insufficient to allow for developing a strategy towards devices with improved lifetime. The support of simulations becomes critical and allows to virtually investigate the effects of many material and stack parameters on the degradation and lifetime of the devices.

2 OLEDdevice lifetime study

In this section, we present a case study showing how 3D KMC simulations can be used to understand and improve OLED devices lifetime.

Introduction

We show how 3D kinetic Monte Carlo (KMC) simulations can be used to study the lifetime of OLED devices and how the insights gained from simulations can quickly lead to the design of devices with improved lifetime. The results are obtained using the advanced simulation software **Bumblebee**, provided by Simbeyond B.V. [1]. The mechanistic character of KMC gives Bumblebee the ability to simulate the degradation of OLED stacks resulting from complex optoelectronic processes. The Bumblebee 3D digital twin of the device (Fig. 1) allows modelers to perform virtual experiments and inspect the device internal behavior with unprecedented detail.

Chemical decomposition of molecular sites is likely triggered by energy dissipation during exciton-exciton annihilation and exciton-polaron quenching events [2-4]. The energy released by these processes is sufficient to cause a molecular site to degrade into one or more products. As a result, molecular sites may become inaccessible to carriers and excitons or, alternatively, electron, hole and exciton traps may form. The properties of the degradation products and their location will determine how the device operation is affected. Moreover, degraded sites can affect the speed at which further degradation develops.

In our study, we explore various degradation scenarios and investigate the impact that different degradation products can have on the device efficiency and lifetime. Simulations were performed under constant current driving, so that the shift in the operating voltage during degradation is obtained. The impact of electron and hole traps formation in different parts of the stack on the voltage-shift and the luminance decay is discussed.

Results

In this work we studied the device that was experimentally characterized by Furukawa et. al in [5]. The simulated stack diagram is shown in Fig. 2. As the first step, we performed a steady state analysis of the device and compared it with the experimental results. The evolution of current density as a function of voltage is presented in Fig. 4. Agood match between the experimental and simulated results at all voltages was found.

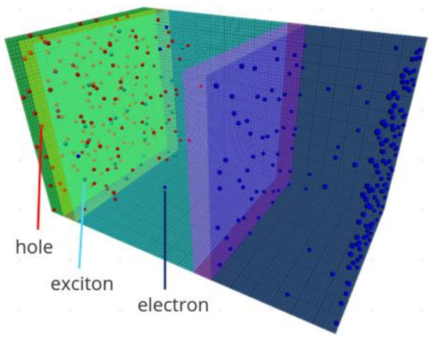

Figure 1. Visualization of a Bumblebee OLED device simulation - Digital twin of the device.
Holes, electrons, and excitons are indicated. Bumblebee simulates charge transport and excitonic processes on each molecular site in 3D. The interplay among all these processes is simulated in time.

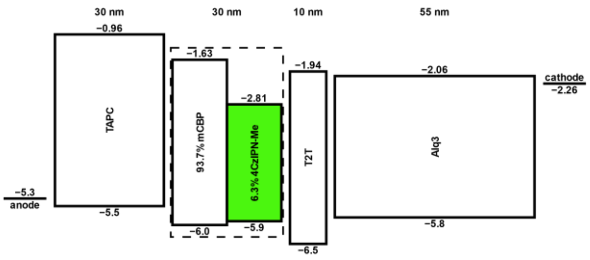

Figure 2. Energy diagram of the simulated stack. Ionization potential and electron affinities of the materials in the layers are displayed.

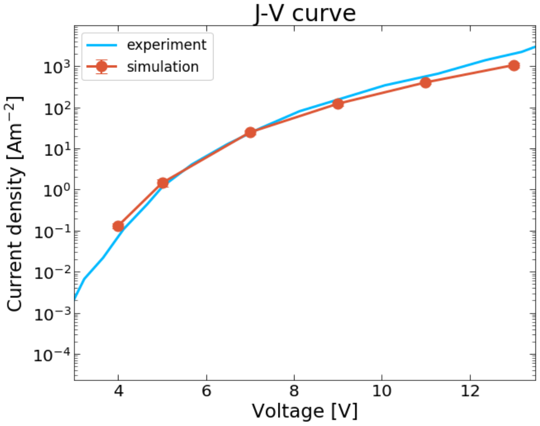

Figure 3. Current density as a function of voltage curve.

Fig. 5 presents the evolution of the External Quantum Efficiency (EQE) as a function of current density. In the absence of a precise light outcoupling profile, the results for the EQE were obtained from the IQE by assuming a constant light outcoupling of 25% at all current densities. This assumption is based on the estimation for the outcoupling efficiency reported in [5]. The results show a good matching between experimental and simulated results both at the lower and higher current densities and less good matching at intermediate values (about 1 Am^{-2}).

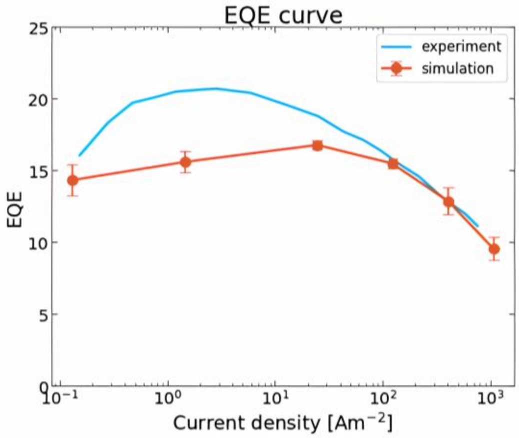

Figure 4. External quantum efficiency curve Assuming a constant outcoupling efficiency in the device of 25%.

Another interesting result that can be obtained with Bumblebee is the contribution of the loss mechanisms to efficiency and roll-off. These results are shown in Fig. 6. The first conclusion that we can draw is that the impact of the non-radiative decay loss remains mostly unchanged at all voltages. On the other hand, we can see that both the quenching and annihilation are getting responsible for most of the losses at higher voltages, which is expected due to higher exciton densities. A result that was not expected is the importance of the quenching at lower operating voltages. This is caused by a charge accumulation at the interface with the EML and a shift in the emission profile at low voltages from the cathode to the anode side of the device, that leads to high exciton-polaron quenching rate at the interface.

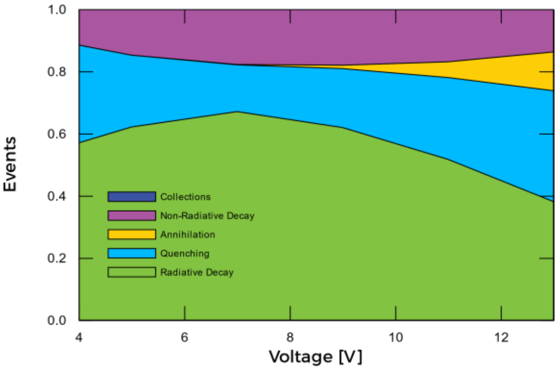

Figure 5. Excitonic events that contribute to the device efficiency and losses at each voltage.

After analyzing the steady state operation of the device without degradation pathways the lifetime of the device can be studied by including the expected material degradation pathways. Fig 7 displays the evolution of radiative rate decay and the voltage shift during degradation of the devices under different degradation scenarios. The influence of different parameters on the device lifetime and driving voltage has been studied. First, we focused only on the degradation of the emitter in the EML and varied the properties of the degraded products. Second, we refined our study including the material degradation in the other layers. Four scenarios for the degraded products were considered. Either the degraded sites became an electron trapping, a hole trapping, a full-trapping site (electron and hole) or a non-trapping inactive site. In our simulations we assumed that materials would degrade with the same probability when a high energetic event like exciton-polaron quenching or exciton-exciton annihilation would happen on the molecular site, Bumblebee simulates the impact of each degraded molecular site on the device behavior. The device operation is simulated in time while degraded products are forming at different locations in the device.

The first conclusion that we can draw from these simulations is that the device lifetime depends strongly on the properties of the degradation product. In particular, we observe that inactive molecular products do not significantly contribute to the decay in light emission (green curve). This suggests that degraded emitter sites must have at least some carrier trapping characters. Simulations predict negligible difference in radiative rate decay between electron and hole trapping degradation products, while a slightly worse lifetime is predicted for this stack when the emitters degrade into fully-trapping sites (yellow curve, electron+hole trapping). On the other hand, enabling degradation of the transport layers in the simulation (in purple) has a mild effect on the radiative rate decay curve when comparing with the scenario where only the TADF emitters can degrade (in yellow). This result is understood by considering that degraded sites in the transport layers mainly affect charge transport, while their impact on the light emission is only indirect.

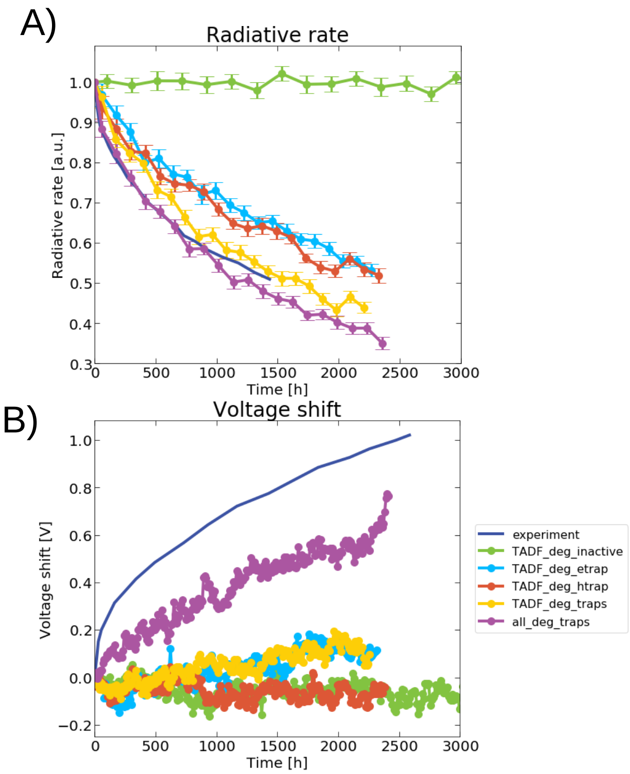

Figure 6. Lifetime prediction for different degradation scenarios. A) decay in radiative rate due to degradation and B) voltage shift during degradation. The degradation products properties are varied.

The relative trends are quite different when looking at the effects on the driving voltage. The voltage shift predicted by Bumblebee shows that both inactive and hole trapping sites cannot be responsible for the voltage shift observed in the experiment. The increase in voltage shift seen in experiment can most likely be attributed to the formation of electron trapping. It is clear however that in the case where the emitter material is the only degrading material in the stack, we cannot fully explain the experimentally measured voltage shift. When the transport layers are included in the degradation scenario, it results in a major impact on the voltage shift. The voltage shift curve obtained with this scenario is getting much closer to the experimentally observed curve suggesting that the degradation of the transport layers has a dominant role in affecting the operation voltage of these devices.

The overall experimental trend is reasonably well reproduced for both the radiative decay rate and voltage shift. However, there is still a quick initial change of the experimental voltage shift curve that is not well reproduced by our modeling.

One may argue that two regimes in the voltage time dependence can be identified: a quick degradation component and a slower degradation component. A possible explanation may be found when considering an extrinsic origin for this effect, such as the presence of water contamination. In fact, water may accelerate the degradation of transport layers up to a certain extent at the beginning of the lifetime measurements. After which, the normal intrinsic degradation mechanisms become dominant. Experimental evidence of this behavior has been reported by H. Yamamoto et. al [6], showing that ultra-high vacuum fabrication of devices with a lower concentration of water contaminants in the stack resulted in a reduced luminance and voltage change during the first stages of device degradation. They argued that electrochemical reduction of water impurities early in the lifetime tests may result in the formation of traps causing a sudden change in the operating voltage that later saturates. This effect might be responsible for the initial drop that is observed in the stack that we studied.

3 Conclusion

In this study, we presented how simulation methods such as 3D KMC can be used for OLED R&D to predict performance and access in depth information about the functioning of the device that is not available with other methods. The mechanistic aspect of KMC allows us to inspect and analyze the subtle contributions that each process has in determining the stack performance and lifetime. The results presented here are only a small example of what can be simulated with the Bumblebee simulation software.

4 References

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