Combining Simulations and Experiments to Study the Impact of Polar OLED Materials

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ETL (Electron Transport Layers) materials often have a non-zero molecular dipole moment. When deposited in an OLED device, this results in a layer with a positive sheet charge density on one side and a negative on the other. So far, only experimental studies have been performed to study the impact of the polarity on the device operation. For the first time we study the effect of polar ETL materials by both electrical characterizations and numerical drift-diffusion simulations. In this contribution we have studied a traditional bi-layer OLED made of TPD and Alq_3.

Previous studies of Brütting et al. [1] have shown that the polar nature of Alq_3 and other polar organic materials induces a typical signature in the capacitance–voltage experiment. Indeed, as we can notice in Fig. 1, two plateaus can be observed in the C-V characterization. Interestingly, the transition voltage (V_{tr}) at which the capacitance changes is strongly dependent on the thickness of the Alq_3 layer. It can be noticed that C-V simulations of such devices, performed with SETFOS 4.1 [2], can reproduce the experimental observation (Figure 1 (b)). In order to simulate the polar nature of the Alq_3, a negative charge sheet density σ=1,1 mC/m^2 was introduced at the interface between Alq_3 and TPD and a positive one at the interface between the Alq_3 and the cathode, this value is in agreement with the one found in [3] using a Kelvin probe. We were able to explain the capacitance vs. voltage characteristic by simulating the hole and electron concentration in the device (not shown here) for $V<V_{tr}$ and $V>V_{tr}$. The validity of our model is also confirmed by low temperature (221-314K) measurements of the capacitance versus frequency of these OLEDs.

Finally, the capacitance vs. voltage was measured after stressing the device with a constant current using PAIOS 2.0 [4]. We notice that the second capacitance plateau tends to disappear as degradation progresses (Fig. 2). This suggests that the effective sheet charge density at the TPD/Alq_3 interface decreases with ageing.

In this contribution we show that polar materials can be simulated using SETFOS 4.1 introducing a charge density sheet on both sides of the polar layer. Capacitance measurements combined with simulations are powerful tools to characterize the physical properties of these materials and their impact on device performance.

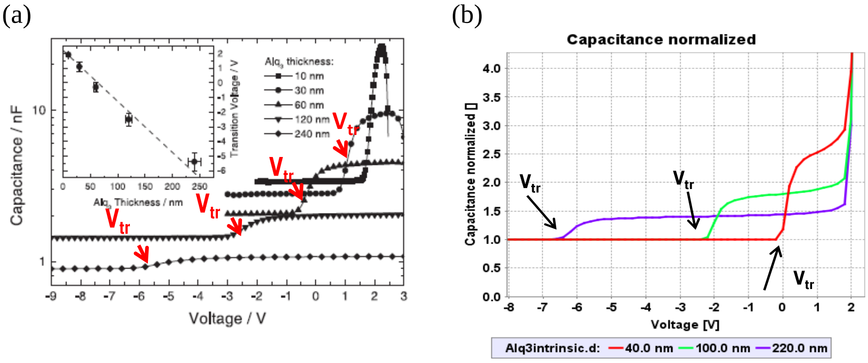

Fig. 1. Measured (a) from [1] and simulated (b) Capacitance-Voltage of OLEDs with different Alq_3 layer thickness using SETFOS 4.1.

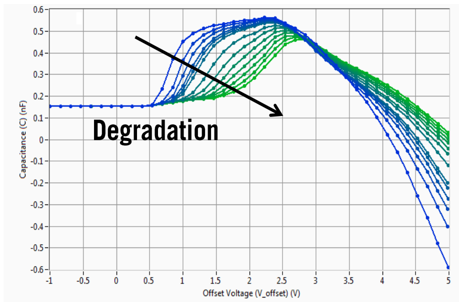

Fig. 2. Measured capacitance versus voltage at different stages of degradation.

References

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4. OLED and OPV characterization platform PAIOS version 2.0 by Fluxim AG, www.fluxim.com, Switzerland .