A conventional 2-layer organic light emitting diode consists of a Hole Transport Layer (HTL) and an electron transport layer (ETL). A good OLED structure requires sufficient carrier injection so that large exciton density is generated when the carriers recombine. However, a 2-layer OLED structure has low injection current due to the poor metal/organic material interface and therefore has low device output efficiency. The electron injection current can be increased by using a different cathode material such as LiF/Al. Unfortunately, LiF/Al metal processing is hard to control and is very sensitive to processing conditions. Also, hole injection is limited by the ITO anode which has large metal/organic barrier.

Recent advances to higher injection current have been made possible by using a p-i-n structure[1] which has high p-doping in the hole transport layer, high n-doping in electron transport layer and a dopant-host emission layer (EML). By selecting the dopant in the EML, red, green and blue OLEDs can be made. The output efficiency can be improved by good metal/organic injection processing.

So far, organic light emitting diode simulations have been used to simulate hole-only or electron-only unipolar devices or simple 2-layer structures. These simple devices can easily be simulated and effects such as hole injection, bulk transport and electron-hole recombination at the HTL/ETL interface can be analyzed. Commercial OLED structures are multi-layer, so it is necessary to understand the basic principles of organic/organic interfaces as well.

In this article, we examine a 3-layer OLED and show why it has a higher device efficiency than 2-layer OLEDs.

### Hole Only Device

As a first step, the basic transport mechanisms are demonstrated using a simple hole-only unipolar organic device. The anode material workfunction is 4.8eV and cathode metals such as Ca, Ag, and Au are frequently used to inject holes. To obtain correct anode Schottky tunneling injection and barrier lowering, the following statements are used:

```plaintext
contact name=anode workfunction=4.8
surf.rec

contact name=cathode workfunction=4.2
surf.rec
```

The Schottky tunneling model is the key to explaining the metal/organic interface injection mechanism.
Multi-layer OLED

To demonstrate why the 3-layer OLED has a higher efficiency than a 2-layer device, we need to understand interfacial effect. The bulk and metal/organic interface can be simulated using the above approach, however organic/organic interface require a different approach.

The main effect of the organic/organic interface is to add trap states which reduces the energy barrier height and enhance the interface energy injection. We used an exponential or Gaussian form for the interface trap states such as equation [1] or [2]. For simulation purposes, we used an exponential form of interfacial trap distribution.

According to ref[3], holes must overcome the barrier height of two adjacent HOMO steps to enter the EML region and either cross the interface or directly recombine with an electron.

The incorporation of the interfacial states lowers the barrier height and so increases the probability of a charge carrier crossing the interface.

For continuous interfacial trap states (organic/organic interface), we used the following statement:

\[
\text{intodefect .s ,s continuous hca=1e20 hcd=1e20 tca=1700 tcd=1700 } \\
y.min<> y.max<> x.min<> x.max<> \
\]

The hca and hcd are for each acceptor-like and donor-like states concentration.

The tca and tcd is exponential decay parameters. The x.min,x.max and y.min,y.max are organic/organic interface coordinates.

Figure 2 shows the IV and VL characteristics with the interface states at the HTL/EML interface.

The device efficiency and luminance have increased.

Figure 3 shows the IV and VL (voltage vs luminance) characteristics without the interfacial states. The 3-layer OLED has a smaller injection current and the same similar output luminance when compared to the 2-layer device.
The luminance in cd/m² is calculated by:

\[ L = \eta \cdot k_m \cdot S \cdot \frac{1}{\tau} \]  \[ \text{[5]} \]

where \( S \) is the integrated exciton density, \( k_m \) is 683 lm/W and the coupling(\( \eta \)) can be calculated either by ray-tracing or the transfer matrix method. User can also directly compare the simulated exciton density profile without detailed optical response of the layers.

Figure 4 shows the Langevin recombination rate and the singlet exciton density for the 2-layer and 3-layer OLEDs. The interface states in the HTL/EML interface result in a lower energy barrier. This increases the hole density at the interface in turn increases the exciton density for the 3-layer device.

Summary

The 3-layer OLED structure has more output efficiency than the 2-layer case. This is because the HTL/EML interface has interface states which lower the energy barrier. This results in increased hole density and exciton density. Despite the fact that the injection is lower than in the 2-layer device, the 3-layer OLED has higher output luminance. If another injection technique, such as a p-i-n OLED, is used then multi-layer OLED will show lower operational voltage and good output efficiency.

References

1. ATLAS User’s Guide, Silvaco, Santa Clara, USA.