https://dx.doi.org/10.22161/ijcmp.3.1.2 ISSN: 2456-866X

A Relatively Complete Description of the Out-coupling Limitation for Planar OLEDs

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Abstract*— *Within this work the computation to describe the out-coupling efficiency limitation of a classical OLED structure is detailed. This manuscript takes a classical geometrical optics approach, combined with fundamental integral calculus. Several specific cases are developed with numerical results. This model looks at the geometrical optics surrounding total internal reflection, including: defining the critical angle, considering the luminous flux distribution at various angles of incidence, and considering the critical angle different materials make with organic layers, ITO, SiNy and air. The critical angles made with typical organic compounds are also studied.

Keywords—geometrical optics, organic light emitting diode (OLED), outcoupling efficiency.

I. INTRODUCTION

There are several key models, of varying complexity, that accurately describe the currently observed out-coupling efficiency values of organic light emitting diode (OLED) devices. These include a classical geometrical optical model, as well as finite difference time domain models. The classical geometrical optics model will be discussed in this work.

The geometrical model makes use of the critical angle associated with each interface in the simple OLED-device structure. A critical angle results from light travelling from a region of high refractive index to a region of low refractive index. It describes the angle of approach with respect to the surface normal of interfaces beyond which all light will be reflected. For light approaching within the critical angle, the Fresnel reflection equations govern the phenomena and incur an additional loss in the extraction efficiency7, however this is neglected due to assumed non-absorption of organic and charge transporting materials. Both of these effects will be considered in the manuscript and quantified in the context present within OLEDs (n).

A. Classical Geometrical Optics Model

Within an organic light emitting diode, the light is generated in a high-index organic layer. The emitted light travels within the organic layer until it reaches the reflecting back contact (on the electron transport side) -typically Al- or travels through organic hole transport layers -typically Indium Tin Oxide (ITO)- and approaches the glass/viewer side. It is assumed in this work that the cathode acts as a perfect reflector and that since the electron transport and charge generating layers are refractive index matched that there is no critical angle present at these material interfaces. The light approaches the interface between the organic and the glass with equal intensities over solid angles. To the author's knowledge, there is no term for this assumption and it will be hereby referred to as isotropically reemitting particles.

The most straightforward models assume that the refractive index is not wavelength dependent over the visible spectrum[1], i.e.:

$$n(\lambda)=n \qquad (1)$$

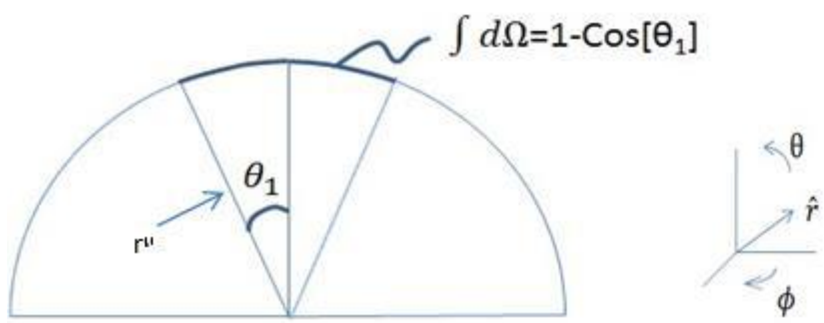

Fig.1: The above figure depicts the relationship between the solid angle subtended by a certain apex angle, θ1, of a cone with radius, r. Integration of Sin[θ] comes from a parameterization of the spherical surface with respect to θ.

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In Eqn. 2, n is a numerical constant specific to a given material. Most materials have a refractive index between 1 and 2.4, but materials such as Gallium(III) arsenide and germanium have refractive indices of 3.92 and 4.01, respectively. The complex refractive index may be measured via spectroscopic ellipsometry[2].

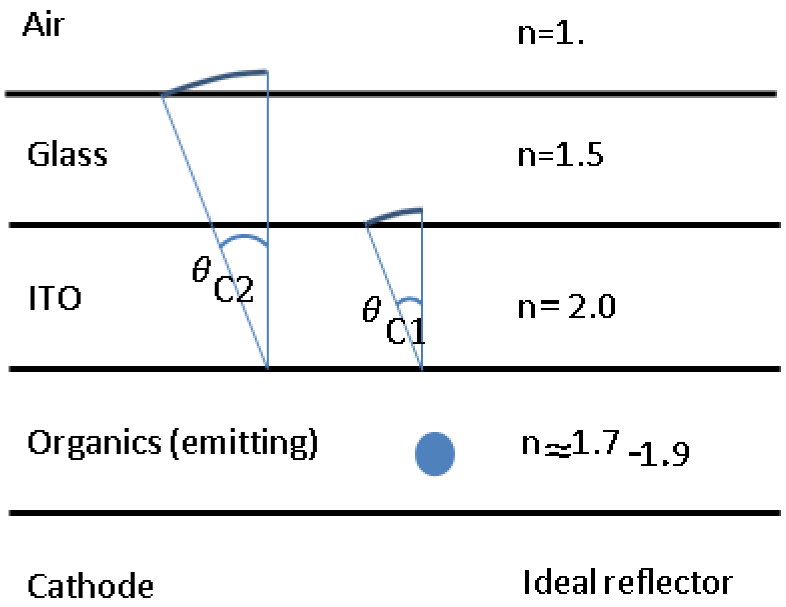
The critical angle is derived from Snell's Law[3]:

$Sin[\Theta_1] \bullet n_1 = Sin[\Theta_2] \bullet n_2$ (2)

To derive the critical angle for a given refractive index ratio, assume that $\Theta_2 = \frac{\pi}{2}$, which

$$\Theta_C = ArcSin\left[\frac{n2}{n1}\right] \quad (3)$$

corresponds to the condition of the light the wave coupling into the surface of the interface and then bending back into the layer it was approaching the dielectric interface from. This is the total internal reflection (TIR) criterion. Then, solve for the θ_1 that would create this condition for a specific set of refractive index ratios and redesignate this angle θ_C. Angles less than θ_C are towards the surface normal and within the exit cone.



The above image depicts a simplified OLED structure. The emitting molecules, one of which is shown, in the organic layer emit light with equal intensity over all solid angles. At each of the organic-glass and glass-air interfaces, there is a critical angle. Rotating the two-dimensional Snell's law criterion about a line directly from the emitting molecule to the planar material interface creates an exit cone. The cathode contact acts as an ideal, non-absorbing reflector of light in this model. Θ_{C1} corresponds to the organic-air exit cone. Θ_{C2} corresponds to the organic-glass exit cone.

The critical angle specifies the maximum angle of approach with respect to the surface normal within which light can escape from medium n_1 to n_2. The trend is that as n_1 increases, the amount of light extracted from the layer decreases.

Since organic materials typically have refractive indices from 1.75 to 1.9[4], and interact with a glass interface of a lower refractive index, a critical angle is introduced. This light will then interact with air. Since glasses have a higher index than air, there is a second critical angle. The smallest of these exit cones defines the extent of reduction in out coupling efficiency (η_C).

The out-coupling efficiency, η_C, will be used to denote the fraction of light that is transmitted across a surface, taking into account corrections for scattering phenomena. In devices without scattering media, this fraction is completely defined by total internal reflection effects. The portion of η_C that quantifies the light escape due to TIR effects will be denoted $\eta_{C,TIR}$. The fraction of the hemispherical solid angle within the escape cone directly equates to the out-coupling efficiency. Assuming a non-dispersive refractive index, then the fraction of light that is able to cross the refractive index interface is the solid angle associated with a unit spherical cap over a cone is given by the following double integral: $\eta_{C,TIR} = \Omega$ (4)

$$\eta_{C,TIR} = \int d\Omega' \quad (5)$$

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$$\eta_{C,TIR} = \int_0^{2\pi}\int_0^{\Theta_C} Sin[\Theta']d\Theta' d\phi' \quad (6)$$
$$= 2\pi(1 - Cos[\Theta_C]) \quad (6a)$$

In this model, there is much more light at the angles that are large with respect to the surface normal. This is obvious when integrating the unit sphere associated with a cone over these angles, where θ denotes the angle from the surface normal. This equation is not valid for theta greater than $\frac{\pi}{2}$.

Next consider the fraction of the solid angle associated with the critical angles for glass-air and organic-glass exit cones. $\eta_{C,TIR}$ for θ_C=41° (the glass-air critical angle) is 24.5% of the hemispherical solid angle, $\eta_{C,TIR}$ for θ_C=59° (the organic-glass critical angle) is 48.5% of the hemispherical solid angle.

A commonly cited method to approximate the amount of light that will be extracted will be to consider the most restrictive exit cone, which is the glass-air one. As stated before, for small molecule, spherical isotropic emitting molecules a first order approximation of the extraction efficiency is given by:

$$\eta_{C,TIR}=\int_0^{\theta_c} \sin(\theta)\, d\theta = 1-Cos[\theta_c] \quad (7)$$

Then, the paraxial approximation- valid for angles less than $\frac{\pi}{2}$for $Cos[\Theta_C]$ is made: $Cos[\Theta_C] = 1 - \frac{\Theta_C{}^2}{2}$. This approximation is valid for the angles of interest. So, $1 - Cos[\Theta_C] = \frac{\Theta_C{}^2}{2}$. Recognizing $\Theta_C = ArcSin[\frac{n_2}{n_1}]$, expand ArcSin[x] as a Taylor Series:

$$ArcSin[x] = x + \frac{1}{2}\left(\frac{x^3}{3}\right) + \left(\frac{1}{2}\right)\left(\frac{3}{4}\right)\left(\frac{x^5}{5}\right) + \left(\frac{1}{2}\right)\left(\frac{3}{4}\right)\left(\frac{5}{6}\right)\left(\frac{x^7}{7}\right) + \cdots$$

Truncating after the first term as an approximation, $ArcSin[\frac{n2}{n1}] = \frac{n2}{n1}$. Then assume n_2=1 for air and the commonly reported literature result is derived[9]:

$$\eta_{C,TIR} = \frac{1}{2\bullet(n_1)^2} \quad (7)$$

Again, n_1 is the refractive index of the organic layer. With n_1=1.75, this gives 18% out-coupling efficiency. It can be shown that for ellipsoidal isotropic emitters, which are molecules in the shape of ellipsoids that emit isotropically, the recently derived approximation can have an n_1 multiplier in the denominator of 1.7; instead of 2. Most organic molecules are more ellipsoidal in shape than spherical.

Other factors that limit the external efficiency of OLEDs are: (i) the lossy, absorptive nature of the aluminum or other back contact and (ii) Fresnel reflections which increase the interactions with the back contact. The absorptions at the back contact are outside of the scope of this work. The lossy nature is due to the imaginary portion of the cathode refractive index in the visible. These factors should reduce the 29% extraction calculated above for n_1=1.75 to the experimentally observed 20% maximum.

It is known that the microcavity effect can be related to the Fresnel reflections and is due to the structure formed between reflecting and opposing surfaces. It plays a role in altering the out-coupling efficiency within the OLED from the derivations presented in this work. To what extent it is enhancing or limiting the out-coupling efficiency in the OLED is not explored within this text.

The microcavity effect is the fact that the waves confined to a small volume of space can interact destructively such that only few resonant modes will be allowed to propagate. It is expected that it does not have such a strong effect on out-coupling efficiency as it does the angular dependence of the emitted light. The viewing angle dependence of the light are dependent upon the size, shape and material characteristics of the microcavity and are readily solvable via the finite difference time domain method and are built into Lumerical FDTD, but are not evaluated in this work.

As a thought experiment, consider the smallest exit cone –the organic-air one- is eliminated, then the organic-glass exit cone becomes the largest obstacle to high out-coupling efficiency devices at 48.5% out-coupling efficiency.

It is important to note the Fresnel reflection effects within the exit cone. For this model, the light within the exit cone will have a certain fraction that gets out due to each pass through the device. With no absorptions in the device, the light has infinite passes to escape and will all get out in the infinite pass limit. (6) Another matter of note is the exit cone from ITO into the organic layers. The exit cone for these layers having index 2.0 and 1.75, as assumed earlier, is 61° as defined by equation (2.3). The fraction of the solid angle within this exit cone is 51.5%. A certain fraction of the light emitted will be outside of the organic-air exit cone, within the organic-glass exit cone but outside of the ITO-organic exit cone. This light will be wave-guided into the edges of the device and is typically referred to as the ITO-glass modes. The difference between 51.5% and 48.5% is 3% that will be trapped in the ITO and the glass and never interact with the cathode.

Within this manuscript it was shown that the classical isotropic emitter model can accurately estimate the experimentally limited out-coupling efficiency (η_C). The Fresnel reflections can be ignored for non-absorptive device media and non-absorbing cathode. The extraction efficiency is defined by 1-Cos[θ_c], where θ_C is the critical angle associated with the organic-air exit cone. For isotropic emitters in a planar structure, the extraction

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efficiency is 29% for organics with index equal to 1.75 and less extraction for higher index materials.

Presently, there is a strong absence in simulations and associated analysis of 3D finite-difference time-domain models of OLED systems. Future studies will aim to close the gap in the literature as well as relax the assumptions made about the lossy nature of the back contact. Furthermore, the magnitude of the Fresnel reflections relative to the total internal reflections will be quantified.

FUNDING

Department of Energy under the National Energy Technology Laboratory Grant # DE-EE0005274.

FUTURE STUDIES

In the future it will be of great import to determine the relevant Fresnel reflection coefficients and an equivalent exit cone within which the reflection coefficient is less than five percent.

ACKNOWLEDGMENT

Thank to Professor Ching Tang and Lewis Rothberg for their advice in the conduct of this research.

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