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Simulation of light extraction from organic light emitting diodes

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Background

• Problem:
  • Poor light extraction efficiency from organic light-emitting diodes

• How to improve it?
  • External quantum efficiency \( \eta_{\text{EQE}} \), which is defined as the ratio of the number of photons emitted to the air and the number of injected charge carriers.
    \[ \eta_{\text{EQE}} = \gamma \times \eta_{s/t} \times \eta_{\rho} \times \eta_{\text{out}} \] (1)
  • The charge imbalance factor \( \gamma \) can be optimized close to 1 by electron and hole transport layers.
  • The ratio of singlet to triplet excitons, \( \eta_{s/t} \) approaches 1 for current phosphorescent materials.
  • The radiative quantum efficiency \( \eta_{\rho} \) represents the ratio of the number of the spin allowed excitons which decay through photon emission to the number of those with nonradiative decay channels through defects. A high \( \eta_{\rho} \) can be achieved by educing defect density.
  • \( \eta_{\text{out}} \)
Background

- The outcoupling factor $\eta_{\text{out}}$ is defined as the ratio of photons emitted to the air side, and all photons emitted inside OLEDs.
- For most organic layers with $n \sim 1.8$, $\eta_{\text{out}} \approx 17\%$
  - Photons trapped in the substrate due to total internal reflection at the glass/air
  - Photons waveguided in the high index organic layers
  - Photons dissipated at the organic/metal by surface plasmons excitation

Figure 1. Simulations for flat OLEDs (wavelength = 530nm)
Background

• Increasing light extraction from bottom-emitting OLEDs
  • The waveguided mode in the substrate can be extracted by scattering centers within the glass substrate or by micro-lens (μLA) arrays at the air-glass side.
  • Internal periodic corrugations can diffract the WG and SP modes, to extract the light trapped in the high-index organic/ITO layers and reduce plasmonic losses
• Our objective
  • Understand the optimal range of pitch and height values for outcoupling
Corrugated OLEDs: Integrated OLED substrates with periodical corrugations. The entire OLED stack is conformally grown on the patterned substrate.

Photons are emitted isotropically by the emissive molecules, with a wave vector that lies on a sphere of radius $k = n_{org} \omega / c$. 

Figure 2. Photon momentum wave vectors emitted inside the OLED
Theoretical Approach

- The parallel component of the wave vector \( k_{||} \) is conserved in a planar OLED.
- Only the small fraction of photons emitted in the narrow air cone outcoupled to air.
- The periodicity can diffract photons with a parallel wave vector \( G \).
  - A waveguided mode within the organic layer can be diffracted back to the air cone and outcoupled when \( k_{||} + G = k_{||}' \) lies within the air cone.

Figure 2. Photon momentum wave vectors emitted inside the OLED.
Scattering Matrix (SM) Approach

- The dipoles emit with amplitude $a^{+}_{\text{inc}}$ and $a^{-}_{\text{inc}}$ in forward and backward directions.
- Then computes amplitudes ($b^{+}, b^{-}$) of the total electric fields for waves propagating in the OLED in the positive and negative directions.
- The scattering matrices ($F$) for the substrate/ITO/HTL stack and the ETL/Ag cathode stack ($B$).
- The fields in the emissive layer are the sum of the incident field $a_{\text{inc}}$ and the total reflected field $b$, traveling in both directions.

Figure 3. Schematic showing the three dipole polarizations in the emissive layer of a flat OLED. Transverse magnetic (TM) modes have electric field (E) in the plane of the figure. The transverse electric (TE) mode has E perpendicular to the plane.
Flat OLEDs

The emitted power within the OLED comes from the three dipole polarizations corresponding to z, x, and y orientations of the dipole:

- Transverse Magnetic Vertical (TMv) Polarization (z-Polarization).

\[
P(TMv) = \frac{3}{2} \int_0^\infty du \frac{u^3}{\sqrt{1-u^2}} \{ 1 + b_i^+ + b_i^- \} \quad (2)
\]

\(u\) is the scaled wave-vector inside the OLED \((u=k_\parallel/(n(\text{org})k_0))\).
Flat OLEDs

• Transverse electric horizontal (TEh) polarization (x-polarization)

\[ P(TEh) = \frac{3}{4} \int_{0}^{\infty} du \frac{u}{\sqrt{1-u^2}} \{ 1 + b_i^+ + b_i^- \} \]  

(3)

• Transverse magnetic horizontal polarization (TMh) modes (y-polarization)

\[ P(TMh) = \frac{3}{4} \int_{0}^{\infty} du \frac{u(1-u^2)}{\sqrt{1-u^2}} \{ 1 + b_i^- - b_i^+ \} \]  

(4)

• We utilize (2-4) for the numerical results for the 3 polarizations (Fig. 2). The total emitted power is

\[ P(tot) = P(TMv) + P(TMh) + P(TEh) = \int_{0}^{\infty} du \ P(u) \]  

(5)
Corrugated OLEDs

• For a periodically corrugated OLED with pitch $a$ and height $h$, the two-dimensional periodic corrugation in the $x,y$ plane is described by reciprocal lattice vectors $\mathbf{G}$,
  - $\mathbf{G}_1 = \frac{2\pi}{a} (1, -\frac{1}{\sqrt{3}})$; $\mathbf{G}_2 = \frac{2\pi}{a} (0, \frac{2}{\sqrt{3}})$.  
  \begin{equation}
  \end{equation}

• Any general reciprocal lattice vector is expressed by $\mathbf{G}(m, n) = m\mathbf{G}_1 + n\mathbf{G}_2$.

Figure 4. Schematic structure of the corrugated OLED in a two-dimensional projection. Three representative positions of the dipole with different heights: low (L), mid (M), and top (T).
Corrugated OLEDs

- The travelling waves inside the OLED have amplitudes $b^+(u,G)$, and $b^-(u,G)$ in the $+z$ and $-z$ directions:
  - $b^+(u,G) = (I - B21F21)^{-1}(B21a^+_{in} + B21F21a^+_{in}) \quad (7)$
  - $b^-(u,G) = (I - F21B12)^{-1}(F21a^+_{in} + F21B12a^-_{in}) \quad (8)$
- The emitted intensity in air is described by the amplitudes $c^+(u,G)$:
  - $c^+(u,G) = F11a^+_{in} + F11(I - F21B12)^{-1}(F21a^+_{in} + F21B12a^-_{in}) \quad (9)$

Figure 4. Schematic structure of the corrugated OLED in a two-dimensional projection. Three representative positions of the dipole with different heights: low (L), mid (M), and top (T).
Corrugated OLEDs

- $H(x)$ are the locations of the dipole in the plane, describing the circular-ring like contours. $H(x)$ has Fourier components $H(G)$:
  - $H(x) = \sum_G \exp(iG \cdot x) H(G)$ (10)

Figure 5. Positions of the dipole emittters in a planar $x, y$ cross section of the OLED. The horizontal polarizations of the dipole (TMh, TEh) and the vertical polarization (TMv) are indicated, with the convention that $xz$ is the emission plane.
Corrugated OLEDs

- The power in the corrugated OLED for the three polarizations is convoluted with the positions of the dipoles in the emissive layer:
  
  \[
  P(TM\, v) = \frac{3}{2} \int_0^\infty du \frac{u^3}{\sqrt{1-u^2}} \{ 1 + \sum_G [b_i^+ (u, G) + b_i^- (u, G)]H(G) \}
  \]
  (11)

  \[
  P(TM\, h) = \frac{3}{4} \int_0^\infty du \frac{u(1-u^2)}{\sqrt{1-u^2}} \{ 1 + \sum_G [b_i^- (u, G) + b_i^+ (u, G)]H(G) \}
  \]
  (12)

  \[
  P(TE\, h) = \frac{3}{4} \int_0^\infty du \frac{u}{\sqrt{1-u^2}} \{ 1 + \sum_G [b_i^+ (u, G) + b_i^- (u, G)]H(G) \}
  \]
  (13)
Corrugated OLEDs

• To simulate the outcoupled power we have generalized the components field $c^+(u)$ for planar OLEDs to the Fourier components $c^+(u,G)$ for corrugated OLEDs.
  
  $\mathbf{P}_{\text{air}} (TMv) = \frac{3}{2} \int_0^\infty du \frac{u^3}{\sqrt{1-u^2}} \{ \sum_{G}^{k_x^2>0} c_{TMv}^+(u, G) \}$
  \hspace{2cm} (14)
  
  $\mathbf{P}_{\text{air}} (TMh) = \frac{3}{4} \int_0^\infty du \frac{u(1-u^2)}{\sqrt{1-u^2}} \{ \sum_{G}^{k_x^2>0} c_{TMh}^+(u, G) \}$
  \hspace{2cm} (15)
  
  $\mathbf{P}_{\text{air}} (TEh) = \frac{3}{4} \int_0^\infty du \frac{u}{\sqrt{1-u^2}} \{ \sum_{G}^{k_x^2>0} c_{TEh}^+(u, G) \}$
  \hspace{2cm} (16)
  
  • The sum over Fourier components $G$ is for propagating modes where $k_x^2 > 0$

  
  $k_x^2 = \left(\frac{\omega}{c}\right)^2 - (u + G_x)^2 - G_y^2$
  \hspace{2cm} (17)
  
  • The total emitted power is

  $\mathbf{P}_{\text{air}} (\text{tot}) = \mathbf{P}_{\text{air}} (TMv) + \mathbf{P}_{\text{air}} (TMh) + \mathbf{P}_{\text{air}} (TEh) = \int_0^\infty du \mathbf{P}_{\text{air}} (u)$
  \hspace{2cm} (18)
Results

We simulate a conformally corrugated OLED with periodic corrugations of pitch $a$ and height $h$.

- The OLED stack is polycarbonate (PC; $n=1.58$)/ corrugations in PC (height $h$ nm, pitch $a$)/ HTL ($d$(HTL) nm)/ emissive region/ ETL $d$ nm /Ag cathode.
- The optimum ETL thickness is a near a quarter wavelength $\lambda/4n$(org), we calculate the average $\eta_{\text{out}}$ for a range of ~20 nm ETL thickness around this value.
- Simulate $\eta_{\text{out}}$ as a function of the corrugation pitch $a$ and height $h$, for three representative wavelengths: 630 nm (red), 550 nm (green), and 480 nm (blue).
Results: Pitch vs Outcoupling for 630 nm

Figure 6. Simulated corrugated OLED outcoupling as a function of corrugation pitch $a$, for a fixed corrugation height $h$ of 200 nm and a red wavelength of 630 nm. The parallel wave vector $k_{||}$ is along $x$, $y$, and $45^\circ$ to $x$ or $y$ axes.
Results: Pitch vs Outcoupling for 550 nm

Figure 7. Simulated corrugated OLED outcoupling as a function of corrugation pitch $a$, for a fixed corrugation height $h$ of 200 nm and a green wavelength of 550 nm. The parallel wave vector $k_{||}$ is along $x$, $y$, and 45° to $x$ or $y$ axes.
Results: Pitch vs Outcoupling for 480 nm

Figure 8. Simulated corrugated OLED outcoupling as a function of corrugation pitch $a$, for a fixed corrugation height $h$ of 200 nm and a blue wavelength of 480 nm. The parallel wave vector $k \parallel$ is along $x$, $y$, and 45° to $x$ or $y$ axes.
Results: Height vs Outcoupling for 630 nm

Figure 9. Simulated corrugated OLED outcoupling as a function of corrugation height h, for a fixed corrugation patch a of 1000 nm and a red wavelength of 630 nm. The parallel wave vector k∥ is along x, y, and 45° to x or y axes.
Results: Height vs Outcoupling for 550 nm

Figure 10. Simulated corrugated OLED outcoupling as a function of corrugation height h, for a fixed corrugation patch a of 1000 nm and a green wavelength of 550 nm. The parallel wave vector $k||$ is along x, y, and 45° to x or y axes.
Results: Height vs Outcoupling for 480 nm

Figure 11. Simulated corrugated OLED outcoupling as a function of corrugation height \( h \), for a fixed corrugation patch \( a \) of 1000 nm and a blue wavelength of 480 nm. The parallel wave vector \( k\parallel \) is along \( x \), \( y \), and 45° to \( x \) or \( y \) axes.
Results: Height vs Outcoupling for 480 nm

Figure 11. Simulated corrugated OLED outcoupling as a function of corrugation height \( h \), for a fixed corrugation patch \( a \) of 1000 nm and a blue wavelength of 480 nm. The parallel wave vector \( k || \) is along \( x \), \( y \), and \( 45^\circ \) to \( x \) or \( y \) axes.
SEMLA

- The dipole emitter has 3 polarizations x (TEh), y (TMh), z (TMv);
- There are inequivalent positions of the dipole emitter:
  - Top position (T) directly above top if pyramid
  - Low (L) position above trough of structure
  - There are positions between T & L
- Mixed layer has polycarbonate/glass index $n_1$ with higher index planarizing material index $n_2$.
- $n_2$ is matched to index of organic layer
- Divide mixed layer $d_2$ into 5 slices with radius $R$, 0.8R, 0.6R, 0.4R, 0.2R

Figure 12. Schematic structure of SEMLA in a two-dimensional projection.
# SEMLA Results: Outcoupling vs Pitch

<table>
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<th>Material</th>
<th>Index $n$</th>
<th>Thickness $d$ (nm)</th>
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<tr>
<td>Polycarbonate n1</td>
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<td>SEMLA n2</td>
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<td>1500</td>
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<tr>
<td>Planar layer n2</td>
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<td>400</td>
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<td>ITO from table</td>
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<td>Org HTL n(org)</td>
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<td>Org ETL</td>
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<tr>
<td>Ag cathode</td>
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</tr>
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</table>

Table 1. Parameters of simulations for SEMLA
SEMLA Results: Outcoupling vs Pitch

Figure 11. Simulated SEMLA outcoupling as a function of corrugation pitch $a$, for a fixed corrugation height $h$ of 1500 nm and a green wavelength of 530 nm. The parallel wave vector $k_{||}$ is along $x$, $y$, and 45° to $x$ or $y$ axes.
Conclusion

- We find periodically corrugated conformal OLEDs exhibit optimal light-outcoupling $\eta_{\text{out}}$ as high as 60-65% over optical wavelengths.
- Optimal pitch values are between 1000-2500 nm, and $\eta_{\text{out}}$ is insensitive to corrugation heights ($h > 100 \text{ nm}$).
- There is a gradual roll-off in $\eta_{\text{out}}$ for larger pitch, and a sharper decrease in $\eta_{\text{out}}$ for pitch values smaller than light wavelengths.
- Near optimal pitch values, periodic corrugations strongly diffract trapped waveguided and plasmonic modes to the air cone, through first-order diffraction.
References:


