Simulation of light extraction from OLEDS with FDTD Solutions

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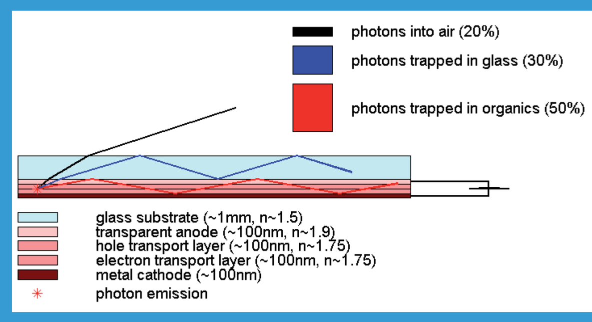
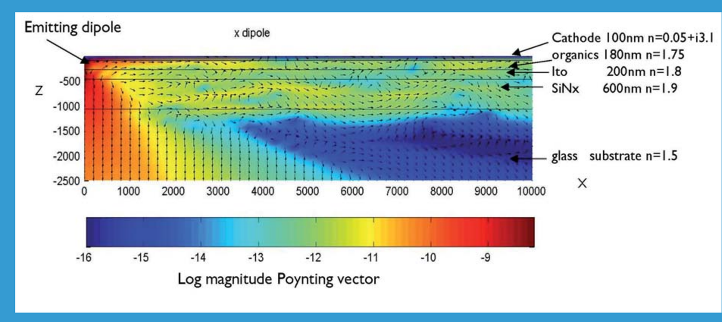
Introduction:

Organic light emitting diodes (OLEDs) consist of thin (50-100nm) electroluminescent organic layers sandwiched between a metal cathode and transparent anode on a glass substrate [1]. They have considerable potential as large area light sources for display and lighting applications. Intense research efforts to improve OLED efficiency, brightness and lifetime are under way worldwide.
OLED light extraction efficiency is limited to about 20% by the high refractive indices of the organic layers (1.7-1.9) and the glass substrate (1.5). Increased light extraction would enable higher efficiency, brightness and lifetime.
About 30% of the generated photons remain trapped in the glass substrate and 50% in the organic layers. Nanophotonic scattering structures close to the emission zone make it possible to tap the "near field" of these "organic modes". This poster shows that these effects can be simulated with the FDTD method [2].



Light trapping in a generic OLED



Waveguiding in an OLED

Modelling light extraction from OLEDs:

In an OLED electron and holes recombine to excitons in the emission zone. The radiative decay of an exciton is described by a classical dipole radiating into the OLED structure and the propagation of light is therefore given by the solution of the Maxwell equations for an oscillating dipole in the layered structure and depends on its location and orientation. The energy flow in the structure and into the substrate is then derived from the electrical and magnetic fields. To evaluate the extraction into the substrate the contributions of many incoherently radiating dipoles with an isotropic angular distribution spread over the emission layer have to be calculated. As OLEDs are broadband emitters the extraction has to be determined as a function of wavelength.

If no scattering elements are present the electrical and magnetic fields of an individual dipole are obtained from the Green's tensor of the layered medium. In the case of scattering the fields are the solution of an integral equation defined on the volume of the scatterers. Its kernel is given by the Green's tensor. The numerical solution poses a number of implementation problems which can be overcome. We observed however that the solutions violated the conservation of energy to an unacceptable degree [3,4,5].

Compared to the integral equation approach the FDTD method conserves energy inherently and furnishes the entire spectral response from one simulation [2]. For large computational domains extending over several wavelengths it requires however considerable computational resources. To meet these demands parallel implementations as provided by the commercial software FDTD Solutions are highly recommendable.

Simulation of light extraction with FDTD Solutions:

FDTD Solutions [6] is a state of the art software which allows to solve the Maxwell equations for complex geometries and gives both time and frequency domain information to the user. It handles a wide variety of material properties including metals. Results obtained in the near field may be transformed to the far-field to obtain scattering patterns. The program can deal with large computational domains spanning many wavelengths due to its parallel implementation (in our work a cluster of 16 state of the art workstations is used). Other notable features are a GUI interface and a scripting language.

To demonstrate the applicability of FDTD Solutions we have chosen an example from the literature [7] and used the following representation in FDTD Solutions:

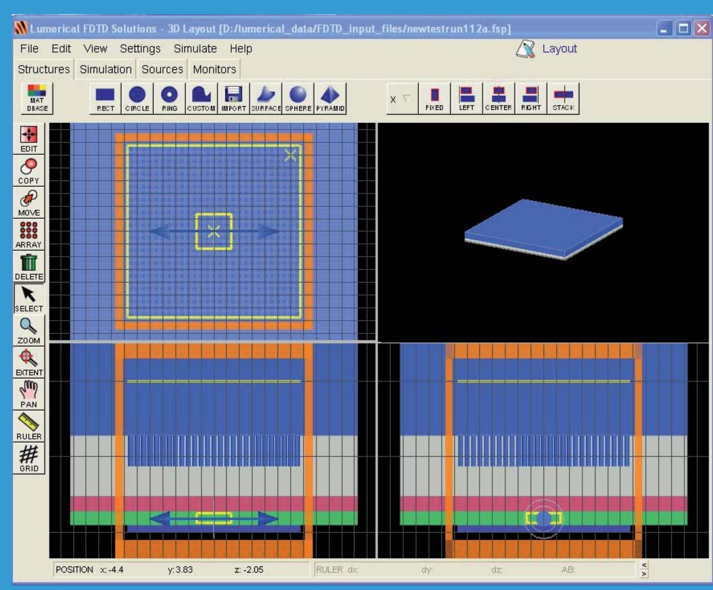
The calculations were performed for a quadratic (L=500nm) and hexagonal grid with the same packing fraction with the following parameters:

Computational volume:	15um x 15um x 2um with PML boundary
Discretization:	dx=dy=25nm, dz=15nm
Broadband excitation pulse:	50 fs
Simulation time:	500fs
Monitor 500nm deep in glass	

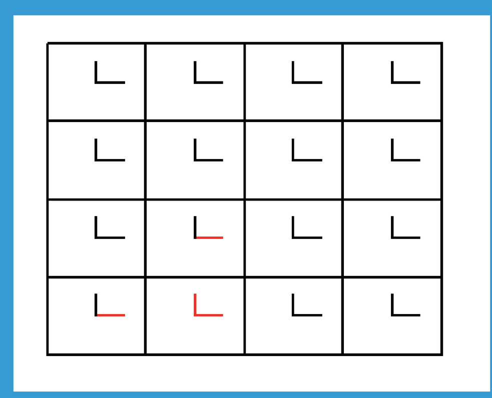
The total memory requirements amounted to about 10GB. A typical calculation for one dipole took about 100min on our system achieving 170Mnodes/sec, i.e. about 10Mnodes/sec per processor. About 90min were needed for the postprocessing (calculation of the far-field distributions as a function of wavelength in steps of 6nm from 400 to 700nm).

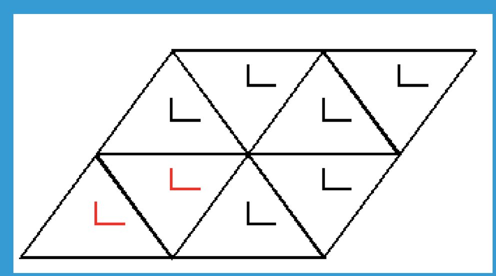
It is straightforward to show that the far-field distribution of an isotropic ensemble of incoherently radiating dipoles at a specific location can be obtained by adding the contributions of three dipoles with orthogonal directions, e.g. x, y and z. The calculation is thus reduced to the evaluation and summation of three orthogonal dipoles in specific locations relative to the scattering structure.

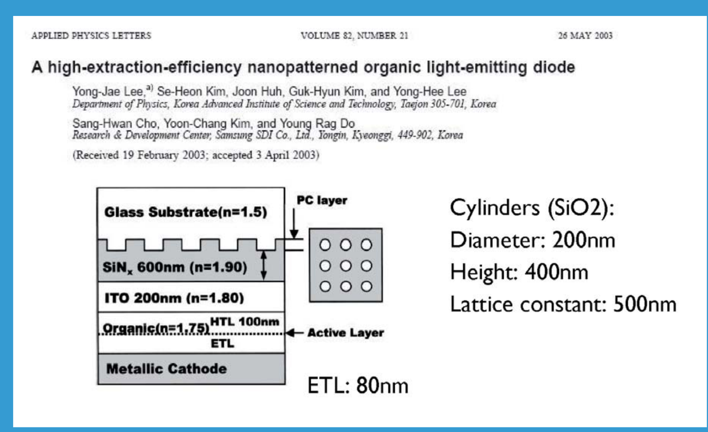
To this end the unit cells were subdivided in subdomains in the center of which the x, y and z dipoles were evaluated. For symmetry reasons only the far-field of the dipoles shown in red had to be calculated. The far-fields of all dipoles were added and the angular energy distribution was derived. These quantities were also calculated for an OLED with identical layers without scattering elements and the relative enhancement of light extraction was determined as a function of wavelength and angle. For the case without scattering the extraction efficiencies and angular distributions were in reasonable agreement with the results obtained with the semi-analytical Green's tensor method.
Furthermore we studied "random" hexagonal lattices where the cylinder positions depart from their ideal positions in a random direction with a maximum distance of 100nm.



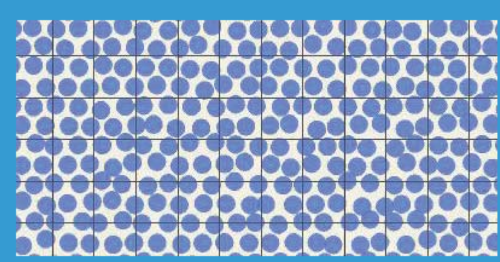
GUI FDTD Solutions


Square unit cell decomposed into subdomains.
Only the dipoles in red have to be calculated


Hexagonal unit cell decomposed into subdomains.
Only the dipoles in red have to be calculated

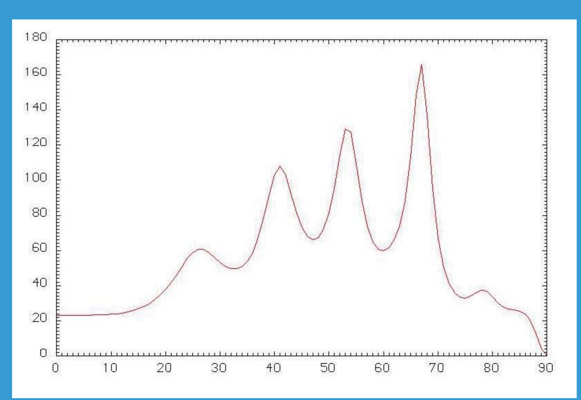


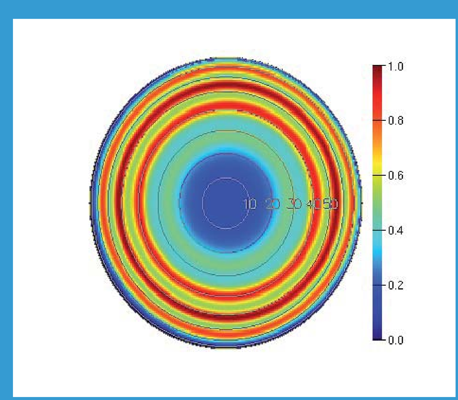
PC (Photonic crystal) like structures for light extraction from OLED

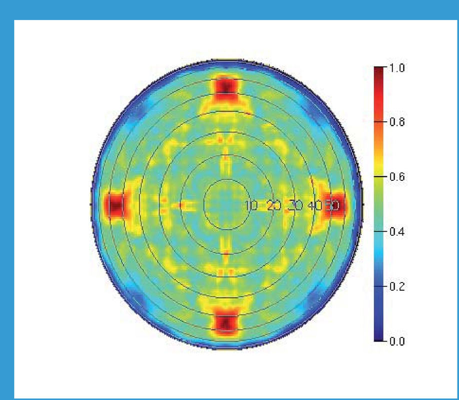

"Random" hexagonal PC

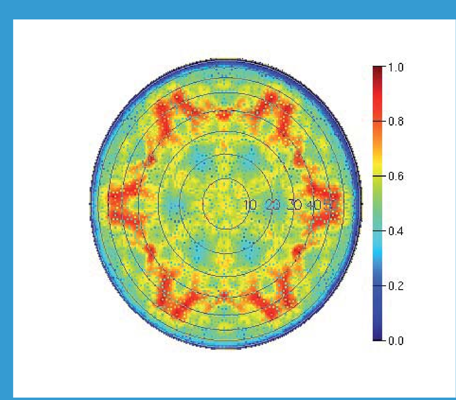
Results:

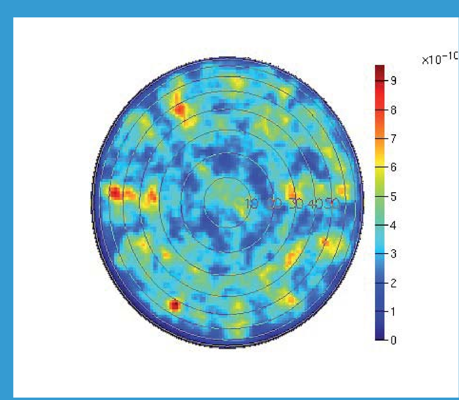
- For OLEDs with no scatterers the FDTD and semi-analytical calculations agree reasonably well (extraction efficiencies, far-field distributions in the substrate) [8].
- By exploiting the symmetries of the problem the calculation can be greatly simplified. The recourse to random pulses distributed in space and time to simulate incoherence is in our experience of questionable validity[9].
- Regular arrangements of scatterers enhance the extraction for certain angles and wavelengths but do not give an overall increase of light extraction into the substrate. Enhancement varies between 1.0 and 1.5 in agreement with experimental observations. Random structures seem to be detrimental.
- The method presented is also applicable to the study of photonic crystals for light extraction in inorganic LEDs

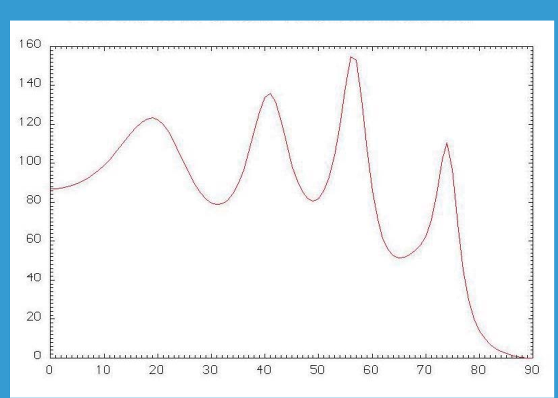

Far-field no PC OLED @ 400nm
(semi-analytical calculation)

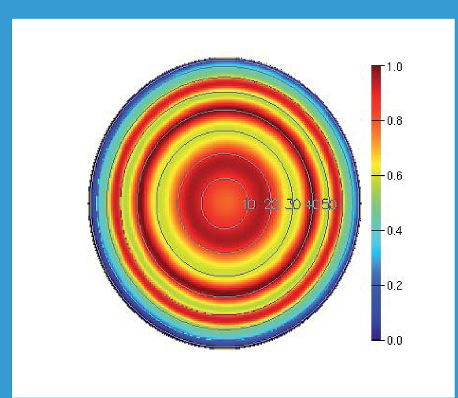

Far-field no PC OLED @ 400nm
(FDTD)

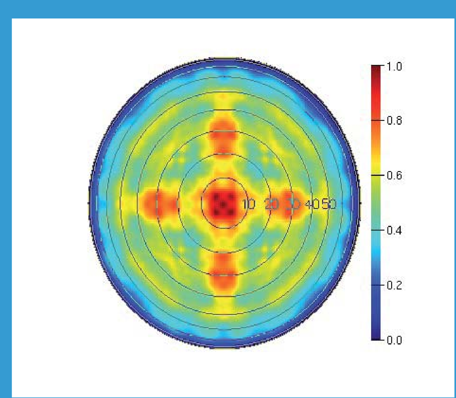

Far-field for quadratic PC @ 400nm

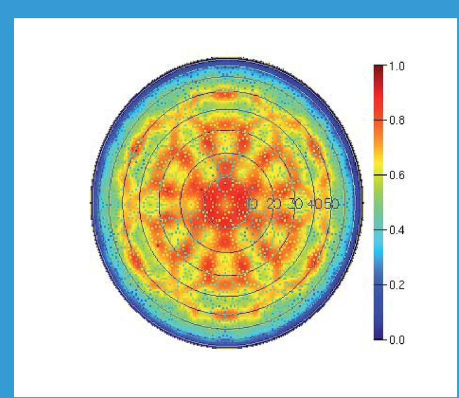

Far-field for hexagonal PC @ 400nm

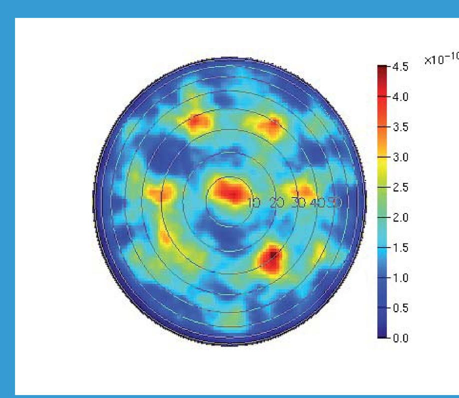

Far-field distribution random PC @ 400nm

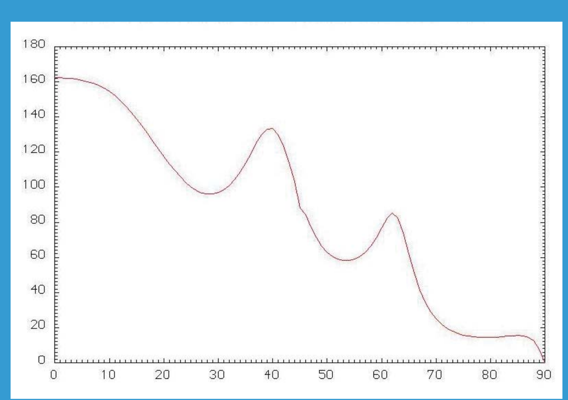

Far-field no PC OLED @ 510nm
(semi-analytical calculation)

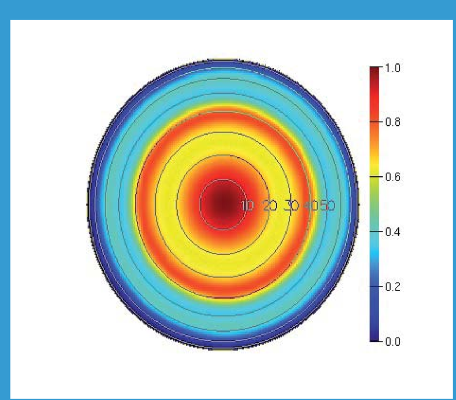

Far-field no PC OLED @ 510nm
(FDTD)

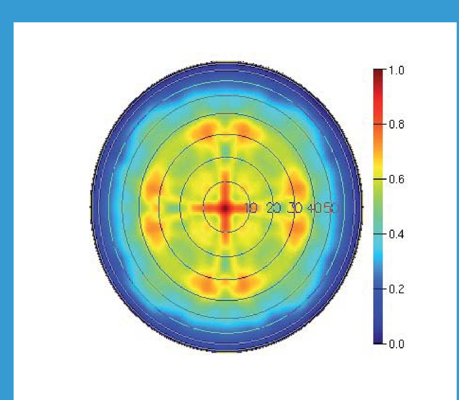

Far-field for quadratic PC @ 510nm

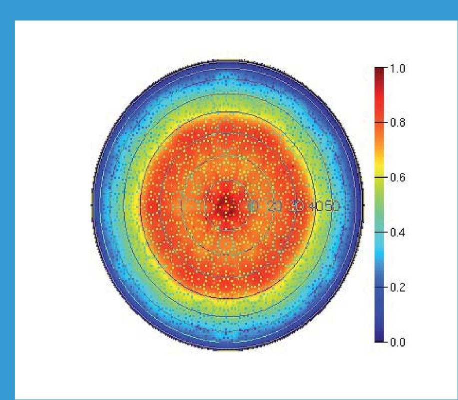

Far-field for hexagonal PC @ 510nm

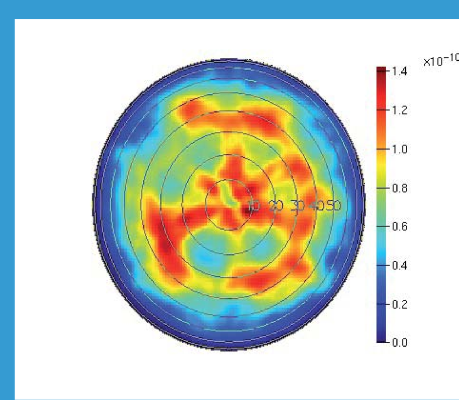

Far-field distribution random PC @ 510nm

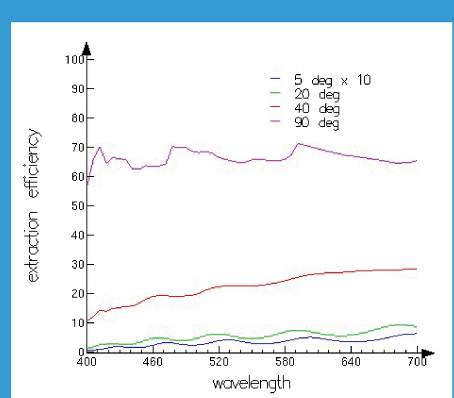

Far-field no PC OLED @ 700nm
(semi-analytical calculation)


Far-field no PC OLED @ 700nm
(FDTD)

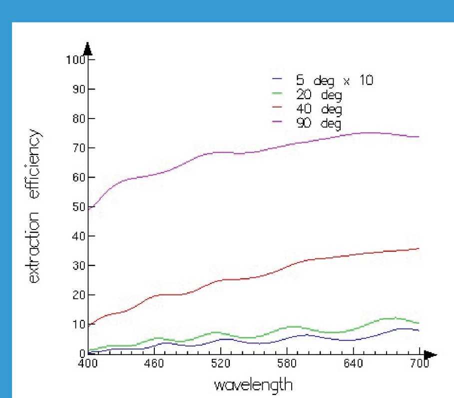

Far-field for quadratic PC @ 700nm


Far-field for hexagonal PC @ 700nm

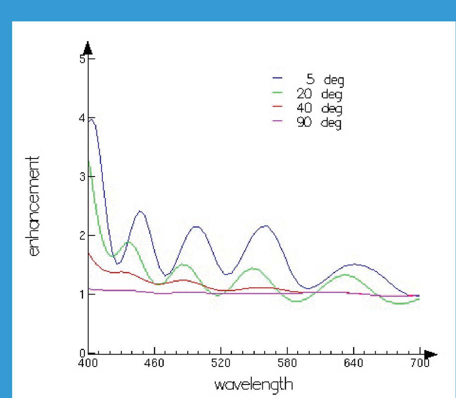

Far-field distribution random PC @ 700nm



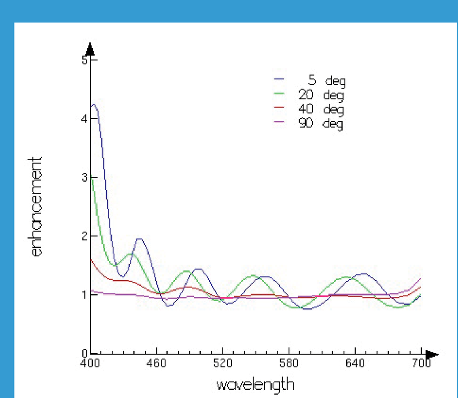
Extraction efficiencies no PC (semi-analytical)



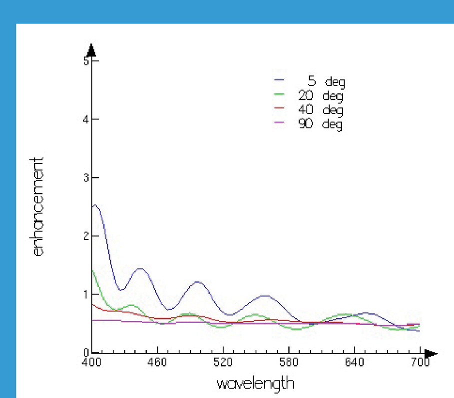
Extraction efficiencies no PC (FDTD)



Enhancement for extraction efficiencies for quadratic PC for various emission cones



Enhancement for extraction efficiencies for hexagonal PC for various emission cones



Enhancement of extraction efficiencies for random PC for various emission cones

Conclusions:

The combination of powerful simulation programs like FDTD Solutions and mathematical insight makes it possible to simulate the effect of scattering structures on the light extraction from organic and inorganic LEDs with reasonable effort and confidence and to elucidate optimal structures for a given problem.

References:

[1] J. Shinar, editor, Organic Light-Emitting Devices – a survey, Springer 2004
[2] A. Taflove, S.C. Hagness, Computational Electrodynamics, the finite-difference time-domain method, Artech House, 2000
[3] H.Greiner, O.J.F. Martin, Numerical Modelling of Light Emission and Propagation in (Organic) LEDs with the Green's Tensor, Proceedings of the SPIE, Vol.5214, pp.248-259
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[5] X. Millard, Q.H. Liu, "A Fast Volume Integral Equation Solver for Electromagnetic Scattering From Large Inhomogeneous Objects in Planarly Layered Media", IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, Vol.51, no 9, pp.2393-2401, 2003
[6] www.lumerical.com
[7] Y.J. Lee et al., "A high-extraction-efficiency nanopatterned organic light-emitting diode", Applied Physics Letters, Vol.82, no.21, 3779-3781, 2003
[8] A. Chutinan et al., Theoretical Analysis on light-extraction efficiency of organic light-emitting diodes using FDTD and mode-expansion methods, Organic Electronics 6, 3-9 (2005)
[9] Y.J. Lee et al., "Far-field radiation of photonic crystal organic light-emitting diode", Optics Express, Vol.13, no.15, 5864, 2005

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