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# Modelling gratings on either side of the substrate for light extraction in light-emitting diodes

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**Abstract** We present a three-dimensional model based on rigorous coupled wave analysis (RCWA) which allows us to study the influence of periodic structures on light extraction in light-emitting diodes. The gratings can be placed both at the interface between the emitting layers and the substrate, where they coherently interact with the dipole field, or at the interface between the substrate and air, where multiple incoherent reflections in the thick substrate contribute to the overall extraction. Even in the case of a grating at the interface between the substrate and air, these multiple incoherent reflections in the substrate still contribute to the overall extraction for large devices, an effect which has been mostly ignored in literature FDTD simulations.

**Keywords** Light-emitting diodes · Gratings · Light extraction · Rigorous coupled wave analysis

## 1 Introduction

In light-emitting diodes (LEDs) emission typically takes place in a high-index layer, meaning that a large fraction of the light is trapped due to total internal reflection, either in the cavity formed by the emitting layers, or inside the substrate. This problem has been studied for a long time in planar layered structures, where the use of microcavities and the optimisation of the planar layer stack were used to alleviate this issue, see e.g. (DeNeve 1995; Benisty 1998a,b).

Another option to increase the light output is to incorporate a periodic structure in the device, which serves to scatter out light that would otherwise be trapped by total internal reflection in high-index layers. This approach has been explored in semiconductor LEDs, see e.g. (David 2006; Delbeke 2002), but also in organic LEDs, see e.g. (Lee 2003; Do 2004).

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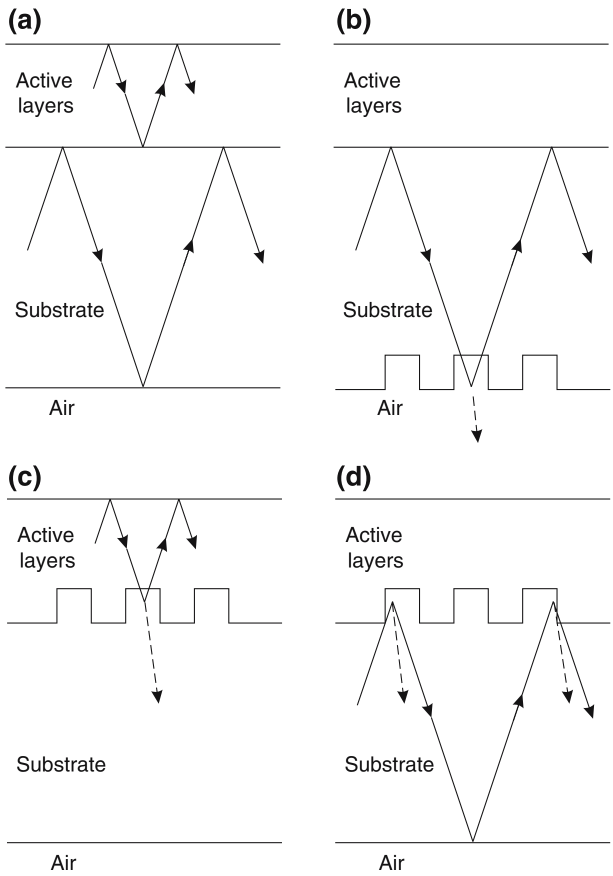


**Fig. 1** (**a**) Light emitted by a dipole in a planar bottom-emitting structure can get trapped either in cavity modes or in substrate modes. The microcavity surrounding the active layer is represented schematically by a single layer, but can of course consist of multiple layers. The figure is not to scale in the sense that the substrate is much thicker than the active layers. (**b**) Placing a grating at the interface between the substrate and air can couple out the substrate modes. A grating at the interface between the emitting layers and the substrate can couple out both the cavity modes (**c**) and the substrate modes (**d**)

When we consider a bottom-emitting structure like the one in Fig. 1, such a periodic structure can be placed either at the interface between the substrate and the air, or at the interface between the active layers and the substrate. A grating at the substrate–air interface can only have an influence on the extraction of the light trapped in the substrate—it has no effect on the light trapped in the cavity surrounding the light-emitting layers at the other side of the substrate. On the other hand, a grating placed at the cavity–substrate interface can have a strong influence on the light trapped in the active layers, and indeed this effect is the main one that has been studied in literature (Lee 2003; Do 2004), mostly with FDTD simulations. However, as Fig. 1 suggests, this grating also scatters the light which is trapped inside the substrate. This can lead to increased outcoupling, as soon as the devices have larger lateral dimensions than a few millimetres, which is definitely the case in large-area tiles of organic LEDs for lighting applications. This effect has been largely overlooked in literature, probably

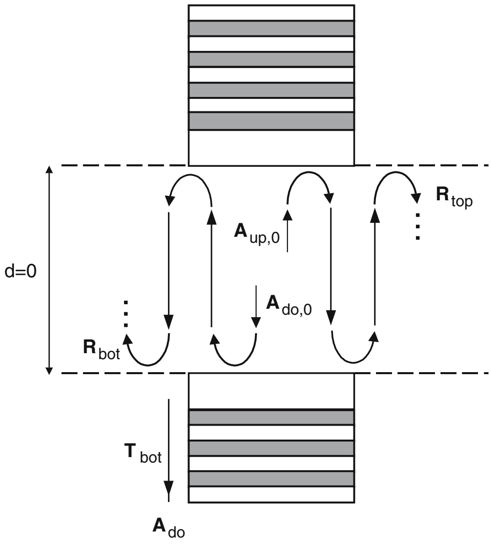


**Fig. 2** Multiple reflections of a source field inside a cavity

because the incoherent effects of a substrate of a few millimetre thickness are difficult to study with FDTD.

In this paper, we expand upon our previous modelling work on grating assisted LEDs (Delbeke 2002), and include the effects of multiple incoherent reflections inside the optically thick substrate.

The rest of this paper is structured as follows. In Sect. 2, we set the stage by briefly reviewing the well-known techniques to model dipole emission in planar layers. Building upon that, we discuss gratings at the substrate–air interface in Sect. 3 and gratings at the cavity–substrate interface in Sect. 4. We illustrate our model with some examples in Sect. 5.

## 2 Planar structures

Spontaneous emission of a dipole in planar structures has been studied for a long time and by several authors (Lukosz 1980; Benisty 1998a,b; Neyts 1998). The basic idea is to take the radiation profile of a dipole and expand it in plane waves:

$$E(\mathbf{r}) = \iint E(k_x, k_y)e^{-j\mathbf{k}\cdot\mathbf{r}}dk_x dk_y \tag{1}$$

The exact expression of $E(k_x, k_y)$ depends of course on the orientation of the dipole and is well-known (Lukosz 1980). If we place this dipole in a layered structure, the radiation profile will change due to multiple reflections of the plane waves making up the source field. The optical environment is schematically depicted in Fig. 2. The horizontal layer containing the dipole separates the upper environment from the lower one, and for each of these we can calculate reflection and transmission coefficients for plane waves, by using Fresnel formulas and an S-matrix scheme.

By combining multiple reflections, we can write for each plane wave the total field at different locations. E.g., for the field that leaves the cavity in the downward direction, we get:

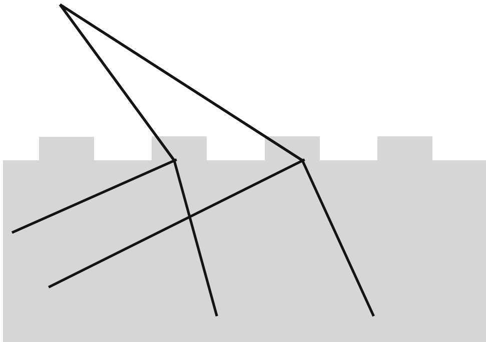

**Fig. 3** An infinitesimal cone representing power flow per solid angle impinges on a grating and schematically results in several transmitted cones. None of the angles in the figure are the same, and therefore also none of the solid angle cones

$$A_{do} = T_{bot} \cdot \left(1 - R_{top} \cdot R_{bot}\right)^{-1} \cdot \left(A_{do,0} + R_{top} \cdot A_{up,0}\right) \tag{2}$$

In this formula, $A_{do,0}$ and $A_{up,0}$ represent the original source fields of the cavity in the downward and the upward direction respectively. $T_{bot}$, $R_{top}$ and $R_{bot}$ are amplitude reflection and transmission coefficients for the plane wave under consideration. $A_{do}$ is the total field leaving the cavity in the downward direction.

By repeating this procedure for all possible angles (or $k$-vectors) contained in the dipole expansion Eq. 1 and integrating the results, we can calculate the total power emitted by the dipole as well as the total power leaving the cavity.

It is important to note here that a plane wave in this formalism is actually related to a density, e.g. in Eq. 1 $E(k_x, k_y)$ refers to a density per unit $dk_x dk_y$. Because of the interest in radiation profiles, it is more conventional to employ a density per unit solid angle $\Omega$:

$$E(\mathbf{r}) = \int E(\Omega) e^{-j\mathbf{k}\cdot\mathbf{r}} d\Omega \tag{3}$$

However, a cone representing a solid angle will be influenced by refraction when going from one medium to another (see Fig. 3). Therefore, when moving from one medium to another, the power densities need to be appropriately rescaled (Benisty 1998a,b).

A final subtlety we want to point out here is that when integrating over all possible angles to get power fluxes, the presence of a guided mode can cause the integrand to become sharply peaked. Therefore, the use of an adaptive integration routine is adviseable.

## 3 Grating at the substrate–air interface

In this section, we want to study the case where the active layer still resides in a planar cavity, but this time a grating is added to the substrate–air interface (see Fig. 1b). The grating is in the most general case two-dimensionally periodic, resulting in a three-dimensional structure. To calculate the bottom emission into air, we proceed along two steps.

First, as far as the initial emission of the dipole into the substrate is concerned, the presence of the grating can be neglected, as it sits on the other side of the optically thick substrate, far beyond the coherence length. Therefore, we can calculate this initial emission into the substrate by using the same methodology as in the previous section, with the exit medium of the bottom half of the cavity being the substrate.

Secondly, this field distribution injected into the substrate is treated as a source term for a second cavity calculation, this time with as top mirror the entire planar cavity with the active layers, and as bottom mirror the substrate–air interface containing the grating.

This second cavity calculation is conceptually similar to the one in Eq. 2, but with a few modifications, To start with, we can no longer restrict ourselves to individual plane waves, but we need to consider a set of plane waves with $k$-vectors related by the Brillouin condition:

$$k_x = k_{x0} + m\Lambda_x \tag{4}$$

$$k_y = k_{y0} + n\Lambda_y \tag{5}$$

Here, $\Lambda_x$ and $\Lambda_y$ are the reciprocal lattice vectors. In theory, we need to retain an infinite number of diffraction orders, however in practise, we limit ourselves to a finite set.

The scalar reflection and transmission coefficients in Eq. 2 now need to be replaced by matrices. We calculate these by using the well-known rigorous coupled wave analysis, making use of the correct Fourier factorisation rules for the product of discontinuous functions (Li 1997).

Another modification comes from the fact that this second cavity formed by the substrate is optically thick, and therefore coherent interference effects cannot take place. This means that the second cavity calculation needs to be performed in terms of powers rather than amplitudes, with power reflection and transmission matrices replacing amplitude reflection and transmission matrices.

A final issue that deserves our attention relates to the fact that the plane waves are to be interpreted as densities. If we adopt the usual convention of working with densities per unit solid angle, the numerical bookkeeping quickly becomes unwieldy, as one input cone now gives rise to *several* output cones, each with a different opening angle (see Fig. 3). An easy way around this problem is to work with densities per unit transverse $k$-vectors $dk_x dk_y$. Indeed, this quantity is conserved across different layers and different diffraction orders, as can easily be seen by differentiating Eq. 4. Therefore, we do not need density conversion factors when power moves from one layer to the next or from one diffraction order to the next.

## 4 Grating at the cavity–substrate interface

Placing a grating at the cavity–substrate interface can have an influence on the outcoupling of both the cavity and the substrate modes (see Fig. 1c and d). We can calculate this in a similar vein as in the previous sections.

First we consider the cavity formed by the active layers and the grating, with the substrate as the bottom exit medium. For this, we use a version of Eq. 2 with matrices and amplitude-based coherent reflections, to calculate the field profile injected into the substrate.

Secondly, this field profile is used a source in the incoherent cavity formed by the grating and the substrate–air interface. This finally allows us to calculate the total extracted power. Note that in FDTD simulations in literature, this second step is not performed, thereby underestimating the extraction efficiency.

It is important to point out that in this case, the extraction efficiency depends crucially on the dipole position with respect to the grating. Therefore, we need to perform several simulations for different dipole positions and average the results. Due to lattice symmetry, considering three positions in high-symmetry points usually already gives us a good estimate of the extraction efficiency.

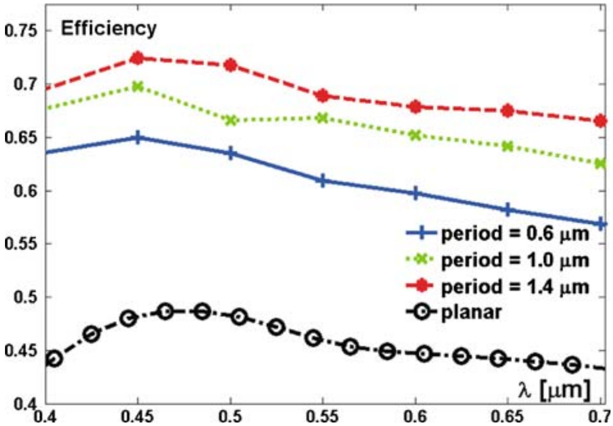


**Fig. 4** Fraction of light injected in the substrate that escapes to the air for an OLED structure with a grating etched in substrate–air interface

## 5 Examples

In this section we will illustrate the model with several examples on organic light emitting diodes on a glass substrate. The code is implemented on top of our eigenmode modelling framework CAMFR (Bienstman 2001), freely available from http://www.camfr.sourceforge.net.

In a first example, we look at a grating at the interface between a glass substrate and air. The diode consists of the following layer stack, starting with the top metal contact: 150 nm Al, 50 nm Alq3, 0 nm emitter layer, 10 nm Alq3, 60 nm NPD, 120 nm ITO, 120 nm SiON, glass. At the other side of the substrate, a square grating of rectangular glass pillars in air is etched. The fill factor of the pillars is 50% and the grating height is 400 nm. Random dipole orientation is assumed. Material dispersion was taken into account using the publicly available refractive index data from SOPRA SA.

In Fig. 4, we show the efficiency of this grating as a function of wavelength and this for different grating periods. Here, the efficiency is defined as the ratio of the light leaving the glass to the amount of light injected in the substrate by the active layers. As such, this figure does not take into account light trapped in the guided modes of the active layers. We see that easily up to 70% of the light injected in the substrate can be extracted, as opposed to only 45% for the case without grating. As a function of wavelength, the behaviour is relatively constant, which indicates that there are no resonant phenomena at work here and the grating functions in essence as a scatterer. The main factor which limits the performance in this case is the loss in the top mirror of the substrate cavity, i.e. the active layer stack. If these layers were to have 100% reflectivity, we would be able to couple all the light out of the substrate. However, mainly due to absorption in the metal, this is not possible. It is also worth pointing out that because of trapping of light in guided modes in the cavity and because of mirror losses, roughly 50% of the total generated light enters the substrate in the first place.

In the second example, we focus on a grating at the interface between the active layers and the glass substrate. This time, the layer stack is 150 nm Al, 85 nm organics with $n = 1.79$, 0 nm emitter layer, 10 nm organics with $n = 1.78$, 10 nm Alq3, 100 nm ITO, 750 nm SiN, a grating layer and the glass substrate. The grating layer consists of square $SiO_2$ pillars in a square lattice in a SiN background. The pillars are 275 nm on the side and the period is 400 nm.

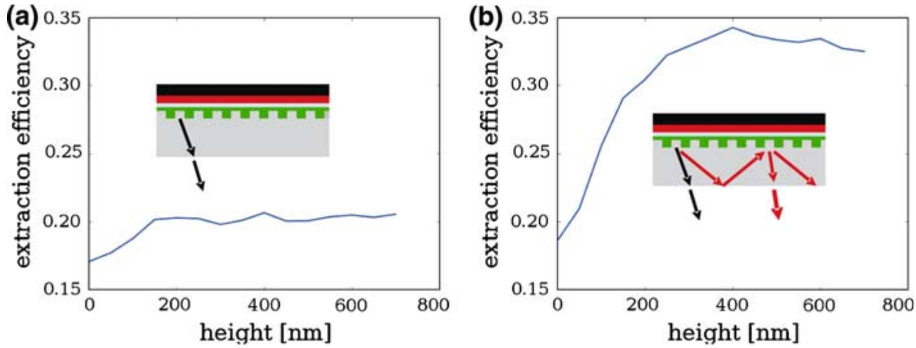


**Fig. 5** Influence of grating thickness on the total light extraction for a grating at the interface between the active layers and the substrate, calculated without (**a**) and with (**b**) multiple reflections in the glass substrate

Figure 5 plots the extraction efficiency at 520 nm as a function of the thickness of the grating layer. The extraction efficiency is defined as the ratio of the power leaving the substrate, to the power emitted by the dipoles in the active layer, i.e. this figure contains both the effects of cavity modes and of substrate modes. Two plots are given, both with and without the multipass effects in the substrate. The figures clearly show that in this case the multipass effects have a significant benefit on the outcoupling performance. Also here, loss in the top mirror is a important factor: the lower this loss, the higher the benefit of multipass effects in the substrate.

## 6 Conclusions

We presented a model to study the influence of gratings on the extraction of light from light emitting diodes. Both gratings at the substrate–air interface and at the substrate–cavity interface can be studied. The model takes multiple reflections into account, coherently inside the cavity and incoherently inside the substrate. The result is a flexible tool to optimise the performance of light emitting diodes with gratings.

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