Highly Efficient Photonic Crystal LED Simulations using Reciprocity

O.T.A. Janssen[1], H.P. Urbach[1]

[1] Delft University of Technology, Lorentzweg 1, 2628CJ Delft, The Netherlands

We calculate the incoherent emission of a periodically structured LED with a highly efficient method based on the reciprocity principle. The method is rigorous, highly parallelizable, and can be run on a desktop PC with any rigorous electromagnetic field solver. Per radiated angle the method requires only two small scattering problems on a single unit cell. With this we obtain the radiated intensity of all possible dipoles at once. The results of the new method are compared to standard LED calculations. Resonances found in the radiation patterns are linked to guided modes of the corresponding 2D photonic crystal.

Introduction

In the last decade, a great leap has been made in producing light emitting diodes (LEDs) that are efficient and bright enough to be widely used. With the onset of high power LEDs, the issue of improving the efficiency has become more important. One aspect is the light extraction efficiency. Due to total internal reflection (TIR) only about 4% of the generated light couples out the top of the LED. In new LED designs, the semiconductor-air interface is modulated by for example photonic crystals to scatter out extra light [1]. In rigorous simulations today, the LEDs are usually approximated by simulating the radiation of many incoherent dipoles that are randomly located and oriented within the active layer of the LED [2, 3]. In practice, a region consisting of a large number of periods surrounding the emitter is discretized. This implies that the calculation of the emission by one dipole requires already a lot of computational resources, let alone the emission by the entire active layer.

In this paper, we demonstrate a method to calculate the radiation of the entire LED in a single direction for any number of incoherent dipoles at any position in the LED, by solving only *two* small quasi-periodic scattering problems on a single cell of the periodic structure. We exploit the reciprocity principle to break up the calculation of the entire radiation pattern of a LED into many small computational problems which can be done on a standard PC. The reciprocity principle is not a new concept, and is already applied in many fields. In [4] it is suggested that the reciprocity principle can be used to calculate the radiation of a single dipole in a planar dielectric stack. It has even already been employed to design a highly directive LED [5].

In the next section, an explanation is given of the reciprocity principle in LED simulations. Thereafter, we show that the reciprocal method can be used to simulate the radiation and improve the design of a photonic crystal LED.

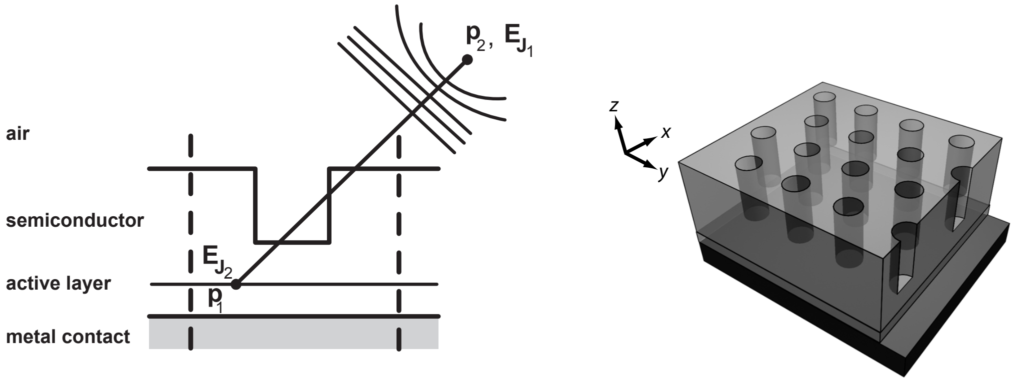

Figure 1: (left) Schematic of a periodic cell of an LED with two dipole sources $\mathbf{p}_1$ and $\mathbf{p}_2$ and their corresponding field observation points $\mathbf{E}_{\mathbf{J}_1}$ and $\mathbf{E}_{\mathbf{J}_2}$ as used in Eq. (1). (right) Schematic of the simulated LED geometry.

Methodology

In classical electrodynamics, a relationship is derived between a time-harmonic electrical current and its radiated field. The relationship remains unchanged if one interchanges the position of the current and the position of the observed electric field. This is known as the Lorentz reciprocity principle, which is given by

$$\iiint \mathbf{E}_{\mathbf{J}_1} \cdot \mathbf{J}_2 \, \mathrm{d}^3\mathbf{r} = \iiint \mathbf{E}_{\mathbf{J}_2} \cdot \mathbf{J}_1 \, \mathrm{d}^3\mathbf{r}. \tag{1}$$

A derivation of this equation can be found in [6]. The theorem is valid for absorbing and anisotropic media, but in general not for nonlinear and active media. The principle links together two situations, namely the electric field $\mathbf{E}_{\mathbf{J}_1}$ caused by a current $\mathbf{J}_1$ and the electric field $\mathbf{E}_{\mathbf{J}_2}$ radiated by the current $\mathbf{J}_2$. Let $\mathbf{J}_1 \equiv -i\omega\mathbf{p}_1\delta(\mathbf{r}-\mathbf{r}_1)$ be the time-harmonic current of a dipole with frequency $\omega > 0$ and dipole moment $\mathbf{p}_1$ at location $\mathbf{r}_1$, and let there similarly be a dipole with moment $\mathbf{p}_2$ at position $\mathbf{r}_2$ as illustrated in Fig. 1a. Because of the reciprocity principle, the electric field emitted in a specific direction by a dipole source can be calculated by calculating the field emitted by a dipole source situated far above the grating in the direction of the emission angle considered. For a dipole 2 far away from the interface, its radiation towards the LED is that of a single plane wave with a polarization determined by dipole moment $\mathbf{p}_2$. The resulting field in the active layer $\mathbf{E}_{\mathrm{near}}(\mathbf{r}_1)$ can be found by solving Maxwell's equations on a single periodic cell. Two scattering problems must be solved, since there are two independent linear polarization states that are perpendicular to $\mathbf{p}_2$. We choose $\mathbf{p}_2^{\mathrm{S}} = \hat{\mathbf{S}}$ and $\mathbf{p}_2^{\mathrm{P}} = \hat{\mathbf{P}}$, with $\hat{\mathbf{S}}$ and $\hat{\mathbf{P}}$ the unit vectors corresponding to the S- and P-polarization respectively. The field $\mathbf{E}_{\mathrm{rad}}(\mathbf{r}_2)$ radiated by dipole 1 in $\mathbf{r}_2$ with arbitrary dipole vector $\mathbf{p}_1$ is then found from the two solutions $\mathbf{E}_{\mathrm{near}}^{S}$ and $\mathbf{E}_{\mathrm{near}}^{P}$ using the reciprocity principle:

$$\mathbf{E}_{\mathrm{rad}}^{\mathrm{S}}(\mathbf{r}_2) \cdot \hat{\mathbf{S}} = \mathbf{E}_{\mathrm{near}}^{\mathrm{S}}(\mathbf{r}_1) \cdot \mathbf{p}_1, \qquad \mathbf{E}_{\mathrm{rad}}^{\mathrm{P}}(\mathbf{r}_2) \cdot \hat{\mathbf{P}} = \mathbf{E}_{\mathrm{near}}^{\mathrm{P}}(\mathbf{r}_1) \cdot \mathbf{p}_1. \tag{2}$$

The total radiated field follows then easily as $\mathbf{E}_{\mathrm{rad}}(\mathbf{r}_2) = \mathbf{E}_{\mathrm{rad}}^{\mathrm{S}}(\mathbf{r}_2) + \mathbf{E}_{\mathrm{rad}}^{\mathrm{P}}(\mathbf{r}_2)$. Because $\mathbf{E}_{\mathrm{rad}}^{\mathrm{S}}(\mathbf{r}_2)$ and $\mathbf{E}_{\mathrm{rad}}^{\mathrm{P}}(\mathbf{r}_2)$ are contributions of incoherent dipoles, the total radiated intensity

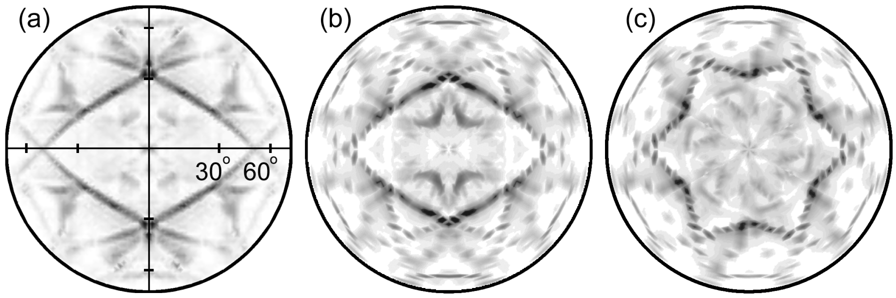

Figure 2: Radiation patterns from (a) a single dipole using the method without reciprocity (b) a single dipole using the reciprocal method, and (c) the entire active layer using the reciprocal method.

in $\mathbf{r_2}$ is proportional to

$$|\mathbf{E}_{\mathrm{rad}}(\mathbf{r_2})|^2 = |\mathbf{E}^{\mathrm{S}}_{\mathrm{rad}}(\mathbf{r}_2)|^2 + |\mathbf{E}^{\mathrm{P}}_{\mathrm{rad}}(\mathbf{r}_2)|^2 = |\mathbf{E}^{\mathrm{S}}_{\mathrm{near}}(\mathbf{r}_1)\cdot\mathbf{p}_1|^2 + |\mathbf{E}^{\mathrm{P}}_{\mathrm{near}}(\mathbf{r}_1)\cdot\mathbf{p}_1|^2. \qquad (3)$$

The intensity at $\mathbf{r}_2$ due to incoherent dipoles at $\mathbf{r}_1$ with random orientation of the dipole vector $\mathbf{p}_1$ is obtained by an integration over the sphere with radius $p_1 \equiv |\mathbf{p_1}|$. Finally, the total intensity at $\mathbf{r}_2$ of randomly oriented incoherent dipoles in the entire active layer O is found by integration over all $\mathbf{r}_1$ in the active layer.

$$I_{\mathrm{tot}}(\mathbf{r}_2) = \frac{p_1^2}{3\pi}\iiint_O |\mathbf{E}^{\mathrm{S}}_{\mathrm{near}}(\mathbf{r}_1)|^2 + |\mathbf{E}^{\mathrm{P}}_{\mathrm{near}}(\mathbf{r}_1)|^2 \,\mathrm{d}^3\mathbf{r}_1. \qquad (4)$$

In conclusion, we have shown that the intensity radiated by the entire active layer in a specific direction can be obtained from the fields obtained by solving only two scattering problems, namely, for two plane waves incident on the periodic structure with S- and P-polarization.

Results

We will apply the reciprocal calculation scheme to a test-case GaN LED as depicted in Fig. 1b. It consists of a 500nm thick layer of GaN on a metallic substrate in air. For the sake of simplicity we assume the metal to be a perfect metal, but this is not a requirement. The active layer is a thin plane 100nm above the metal substrate. The top of the GaN layer is corrugated by a 2D photonic crystal of 300nm deep air columns in a triangular lattice with lattice constant a. We assume dipole radiation at a wavelength of 400nm.

First, the radiation pattern of a single dipole is simulated using the method without reciprocity discussed in the introduction. A domain consisting of size $64a \times 64a$ with $a = 250nm$ is discretized and a single dipole source directed along the x-axis excites the grid. From a Fourier transform of the field just above the GaN layer the radiated far field for this single dipole and is determined and plotted in Fig. 2a. The simulation used 80GB of memory and took over 500 hours of computing time (for a single processor).

Plotted in Fig. 2b is the radiation pattern of a single dipole as simulated with the reciprocal method. Each point in the radiation pattern, follows from two small scale rigorous computations. Because of symmetry we only need to take into account $1/12^{\mathrm{th}}$ of all the angles. Each simulation took about 10 minutes and used 70MB of memory, so that in total

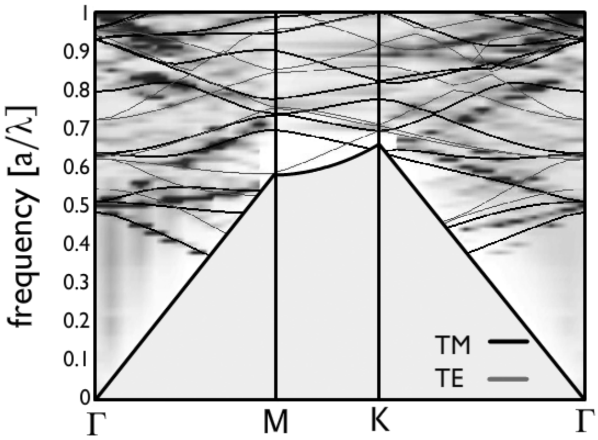

Figure 3: Optical band diagram plotting radiated intensities of the LED, the lines are the modes of the 2D photonic crystal calculated with [7]

40GB and 100 hours were needed. This is still substantial. However, unlike the method without reciprocity, the data from these simulations also give the combined radiation of all incoherent dipoles in the entire active layer, see Fig. 2c.
To better understand the sharp resonance lines in the radiation patterns, simulations were performed for many different lattice constants and at angles corresponding to the edge of the first Brilliouin zone. In Fig. 3a, the results are plotted in a band diagram. It is clear that the sharp resonances correspond to some of the guided modes of the 2D photonic crystal.

Conclusions

We employed the reciprocity principle to simulate LED radiation in a highly parallelizable manner. The main feature of this method compared to other methods is that only two small-scale simulations are needed to obtain the contributions of all incoherent dipoles in the active layer at the same time. The outcoupling problem transforms to an incoupling problem that can be addressed by finding guided modes of the structure.

References

[1] A. David, H. Benisty, and C. Weisbuch. Optimization of Light-Diffracting Photonic-Crystals for High Extraction Efficiency LEDs. *J. Display Technol*, 3:133–148, 2007.

[2] W.J. Choi, Q.H. Park, D. Kim, H. Jeon, C. Sone, and Y. Park. FDTD Simulation for Light Extraction in a GaN-Based LED. *Journal of the Korean Physical Society*, 49(3):877–880, 2006.

[3] Y.J. Lee, S.H. Kim, G.H. Kim, Y.H. Lee, S.H. Cho, Y.W. Song, Y.C. Kim, and Y.R. Do. Far-field radiation of photonic crystal organic light-emitting diode. *Optics Express*, 13(15):5864–5870, 2005.

[4] C.E. Reed, J. Giergiel, J.C. Hemminger, and S. Ushioda. Dipole radiation in a multilayer geometry. *Physical Review B*, 36(9):4990–5000, 1987.

[5] A.L. Fehrembach, S. Enoch, and A. Sentenac. Highly directive light sources using two-dimensional photonic crystal slabs. *Applied Physics Letters*, 79:4280, 2001.

[6] L.D. Landau, E.M. Lifshitz, and A.L. King. Electrodynamics of Continuous Media. *American Journal of Physics*, 29:647, 1961.

[7] S. G. Johnson and J. D. Joannopoulos. Block-iterative frequency-domain methods for maxwell's equations in a planewave basis. *Optics Express*, 8(3):173–190, 2001.