CrystalWave TECH NOTE

Calculation of the extraction efficiency of an LED

Klearchos Chaloulos

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Abstract: We will demonstrate a procedure to model and calculate the extraction efficiency of an LED. First we will study a simple LED, measure the extraction efficiency using CrystalWave and compare the result to the one expected from theory. Then we do the same measurement for the case of an LED etched with a photonic crystal. We describe how modelling the photonic crystal LED with periodic walls can be used to overcome memory limitation problems.

1.1 Introduction

The extraction efficiency is a very important parameter of an LED. It is defined as the ratio of photons escaping the device to the number of photons generated in the device. Its value is often low mainly limited by total internal reflection (TIR). We will measure the extraction efficiency by first exciting a dipole field in the active layer of the device, then measuring the power generated by the dipole and comparing with the power escaping the device.

It should be noted that in this way the device is assumed passive and we are measuring its passive response to the electromagnetic field generated inside it. We do not attempt to measure the spontaneous enhancement (Purcell effect) due to e.g. a resonant cavity. Through the Purcell Effect, the electromagnetic environment in the LED interacts with the quantum mechanical oscillators that are about to emit photons, and guides them to preferentially emit photons in a specific mode of the resonant cavity. If this mode has high extraction efficiency, the overall efficiency of the LED will increase.

1.2 Structure

The structure can be seen on Fig 1. There we plot the epitaxial growth profile of the device. It consists of Sapphire substrate, on which GaN is grown. On top is air. The place where light emission occurs is called the active layer. It is in the middle of this layer that we place out dipole excitors. We will do three different simulations, each with a different (X, Y or Z) polarisation of the dipole excitor. Then we will average the results.

To get quantitative results about the extraction efficiency, we need to measure the dipole power, and the useful power exiting the device. The latter in this case is simply the power (flux) going through the Top sensor. To measure the dipole power there are two ways. One is to enclose the dipole in a small "box", consisting of six sensors. Then the total injected power is the sum of the net flux (net power going out) of these six sensors. Alternatively, we can enclose the whole device with a big box ("BigBox"), consisting of six big sensors. If there is no absorption, and there is enough time for the pulse to propagate and pass through the sensors, then the sum of the net fluxes should give us the total injected power. Obviously, the Top sensor is a part of the BigBox also. The advantage of the BigBox is that the net flux calculations will be more accurate, as it will not be influenced by reflections travelling within the device. Such reflections might travel through the small box many times and disrupt its net flux measurement. The advantages of the small box are that it can be used with absorption and uses less memory.

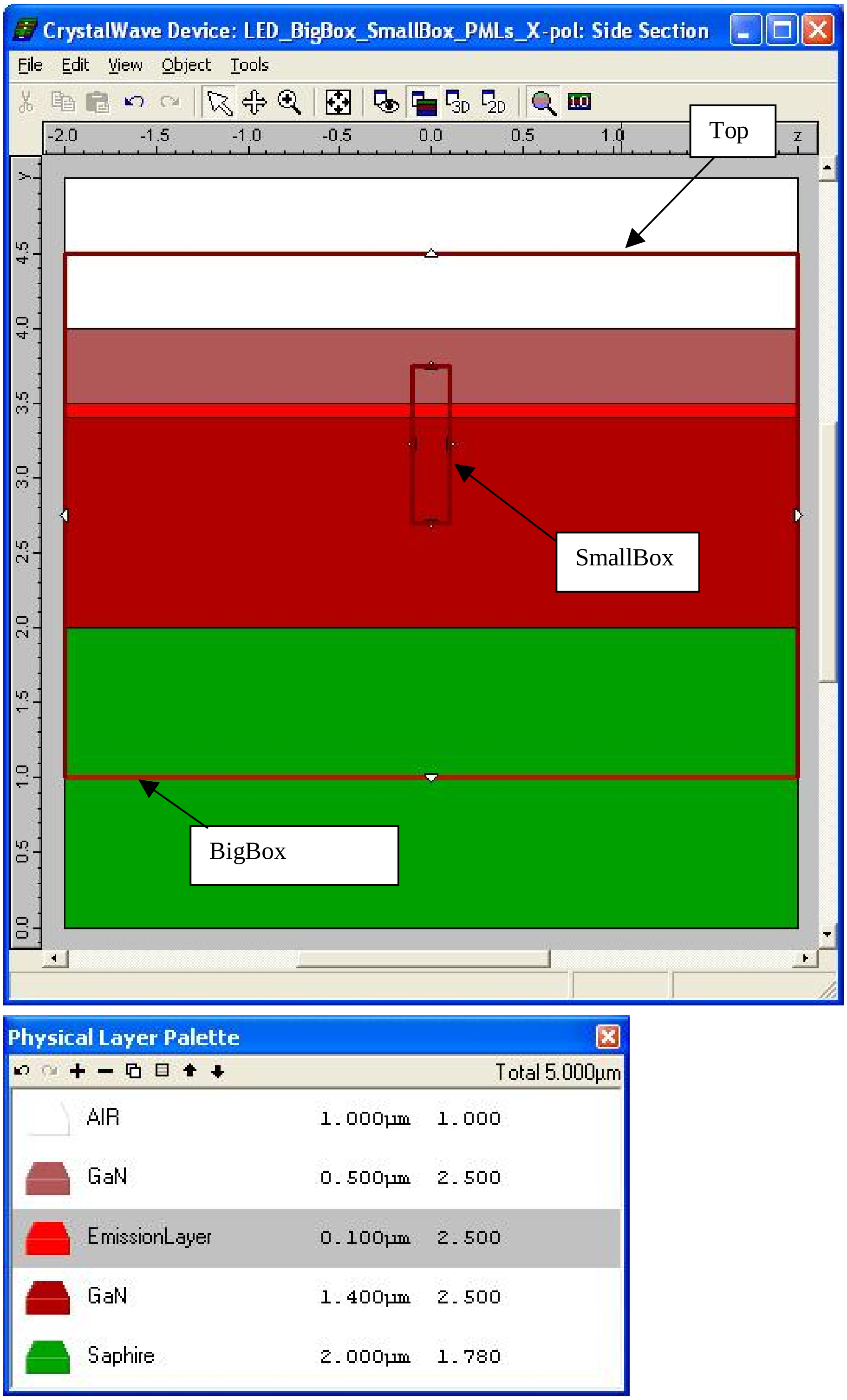

Figure 1: Epitaxial Layer structure of the device. From here, we can see the Sensors forming the BigBox and the SmallBox.

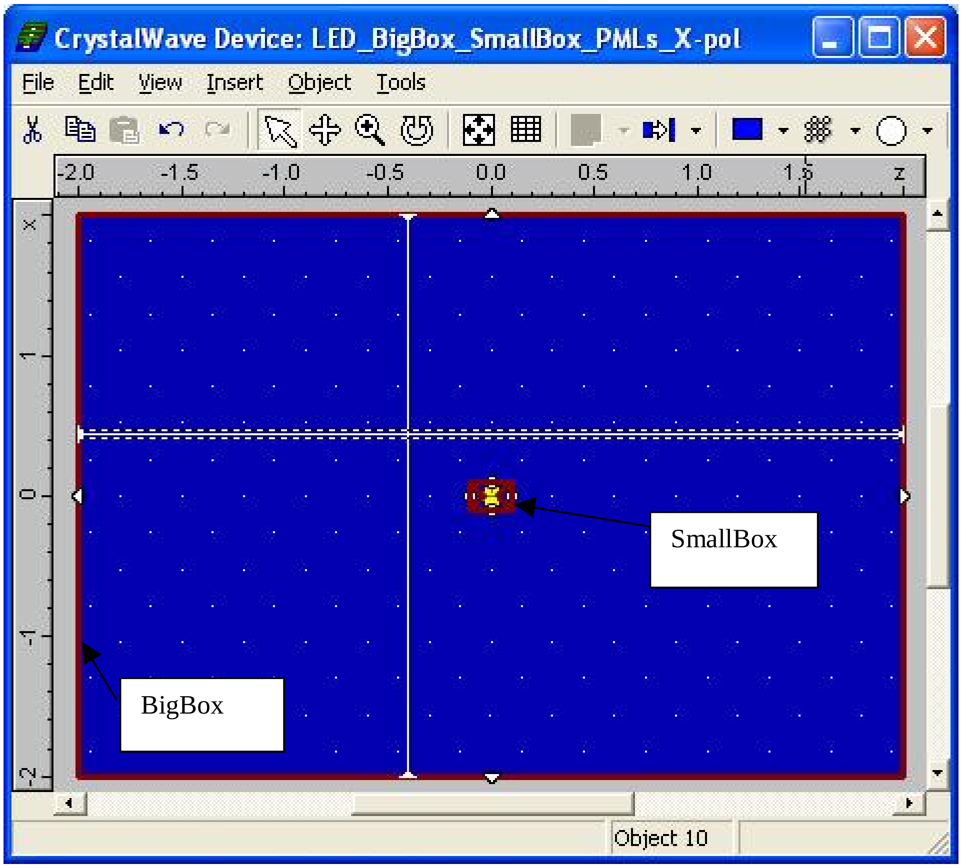

Figure 2: Top view of the device.

The top view of the device can be seen in Fig. 2. The lateral dimensions of the device in the case of the plain structure are not that important. However, Fig. 3 illustrates a point of which we must be careful. We can see that there is some power radiated from the top of the device, but at a very steep angle. This power will not pass through the Top sensor but from the sensor on the side. Evidently this will decrease the extraction efficiency, so the user must make sure that the device is big enough and the Top sensor close enough to the radiating surface, so that this power is not significant.

The sensors of the BigBox are large and they might occupy a lot of memory in the frequency domain. We can get around that if we use the SensorIntegrateFlux feature. This feature integrates the flux through the sensors in the time domain, so no memory in the Frequency domain is needed. We can reduce the memory in the frequency domain, by using a very large value for the SensorTimeUndersample parameter (Fig 4). This comes with the disadvantage that we will not be able to calculate extraction efficiency vs wavelength, but usually extraction efficiency is defined as the total number of photons coming out, with no respect to wavelength. If extraction efficiency vs wavelength is necessary, then we may have to use the small box approach to conserve memory.

Another approach is to surround the structure with periodic walls. This has he disadvantage that it will simulate only waves that satisfy the phase matching conditions at the boundaries of the simulation. This might lead to the extinction e.g. of a resonance, if its spatial profile does not satisfy these boundary conditions. It has however the advantage that the simulation area can be made very small. In addition, the problem of useful output power leaking through the side sensors is eliminated. It should be noted that the power that is confined in the high index layer via Total Internal Reflection (TIR), will stay there and never escape or decay, if periodic walls are used.

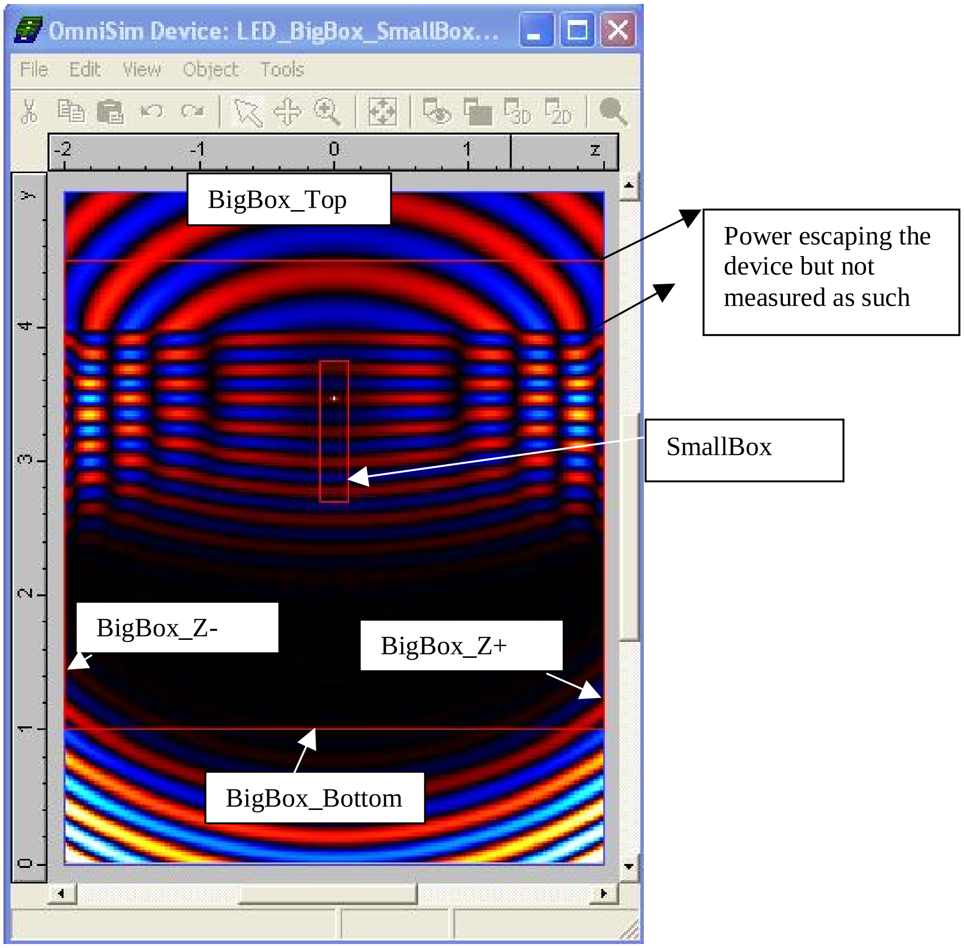

Figure 3: Power escaping the device from Top, but not measure d as one. To fix this, one can do two things: 1) Bring the Top sensor lower, closer to the interface, 2) Make the device wider.

Plain Structure Results

Before we proceed to the results of the simulations, we will try to estimate theoretically the extraction efficiency of a planar structure. Ignoring any resonance or modal effects, we will model the extraction process with a ray picture. Then the only mechanism that stops light from going out is TIR. In our case the critical angle between a layer of index 2.5 and air is θ_C=23.58deg or 0.41rad. The solid angle created by the rotation of an angle θ is $\Theta = 2\pi(1-\cos\theta)$. The total solid angle is 4π. Therefore, if we ignore the transmission dependence on angle and polarisation, we can say that the extraction efficiency is

$$\eta = \frac{2\pi(1-\cos\theta_c)}{4\pi} = \frac{1-\cos\theta_c}{2} \qquad (1)$$

For our example, the extraction efficiency would be about 0.0417 or 4.17%. Because in this calculation we assumed transmittance of 1 below the critical angle, the actual extraction efficiency will be lower. For example the reflection at normal incidence for this interface is 018.3, and it increases with increasing angle, so we should expect an extraction efficiency at about 0.75*η=0.313 or 31.3%.

The calculated extraction efficiencies can be seen on Table 1. We see that we get very good agreement with theory, as the average extraction efficiency is about 3%. The simulation with the periodic walls seems to agree reasonably well with the PML simulations. In addition, note the slight rise in the extraction efficiency when we increased the size of the simulation from 4um to 6um.

Table 1: LED extraction efficiency. We see good agreement between the different methods of simulation, and with the expected approximate value from theory. The devices with PMLs are in sub project "Plain Structure PMLs", while devices with period walls are in subproject Plain Structure Periodic Walls.

	PMLs, Plain Strucxture, 4umx4um	
Polarisation	Top Efficiency Big Box	Top Efficiency Small Box
X	0.044529384	0.045108202
Z	0.044713869	0.045325362
Y	0.004260003	0.004302185
Average	0.031167752	0.031578583
	PMLs, Plain Strucxture, 6umx6um	
Polarisation	Top Efficiency Big Box	Top Efficiency Small Box
X	0.04461032	0.047356634
Z	0.045990682	0.046659847
Y	0.004544295	0.004580666
Average	0.031715099	0.032865715
	Periodic Walls, Plain Strucxture, 1umx1um	
Polarisation	Top Efficiency Big Box	Top Efficiency Small Box
X	N/A	0.043024414
Z	N/A	0.042601904
Y	N/A	0.003286248
Average	N/A	0.029637522

Photonic Crystal Results

In this section we will add photonic crystal to the LED and compute its extraction efficiency. If the photonic crystal is of the right design, it can significantly enhance the extraction efficiency of the LED. The photonic crystal in our example has a square lattice, a period of 0.3um, square holes of radius 0.1um and etch depth of 0.2um. The structure can be seen in Fig. 4.

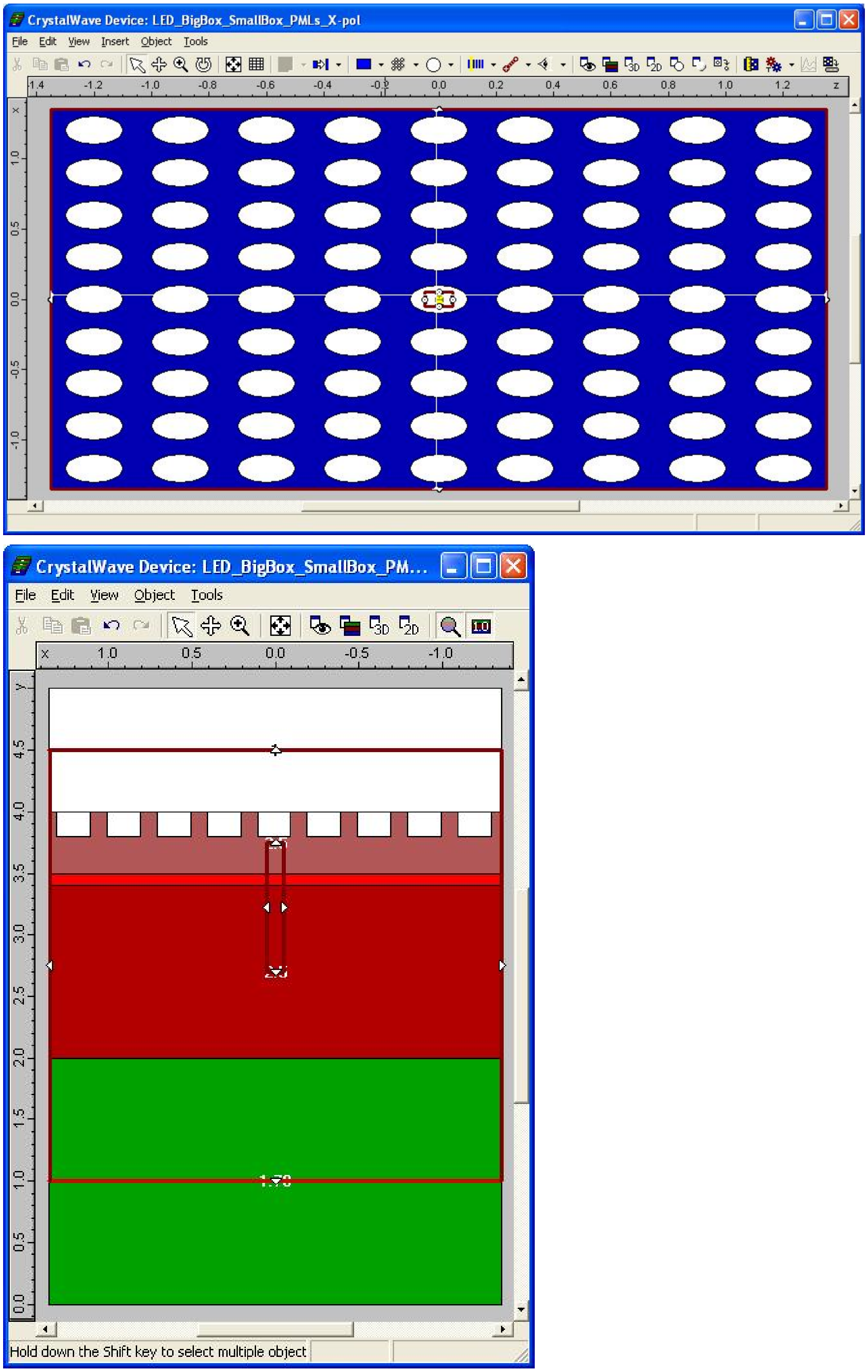

Figure 4: Top view (top) and cross section (bottom) of the device with photonic crystal. Device is LED_BigBox_SmallBox_PMLs_X-pol in sub-project Photonic Crystal PMLs. We see that the sensor configuration is the same as in Fig. 1.

When we use the photonic crystal, another question comes up, what should the size of the device be? The straightforward approach would be to make the device as big it would be in reality. However, usually LEDs are at least several tens of microns long and wide, so that would demand an enormous amount of memory. One approach is to use periodic walls. The idea is to explore the periodicity of the structure. Therefore, you create a structure, which has dimensions equal to an integer number of periods. Then you set the lateral boundaries (X, Z in the case of Fig 4) to periodic, and you will model an infinite extension of the structure. The problem is that this imposed periodicity restricts the allowed solutions of Maxwell's equations. So the actual structure will be able to support more modes than the one with the periodic walls. This effect is more important the smaller the simulation area is.

The other parameter you need to think about is the duration of the simulation. When there is no photonic crystal, all the light that travels above the critical angle will stay in the high index layer. With the photonic crystal, all the light will eventually escape or be absorbed if there is absorption. Therefore the longer the duration of the simulation, the higher the efficiency you will get. That is if there is no absorption. Also, light that travels in the high index layer will reach the boundaries of the device and scatter away. In many cases, this is not useful, as e.g. if the device is a pixel in a camera. Therefore, the duration of the simulation should not be much greater than the time light needs to reach the edge of the pixel. So if you use periodic walls, you ca model the size of the device indirectly by setting the duration of the simulation to the time light needs to reach the boundaries of the device (of course this is an approximation). In this example, we will use some fixed duration and no absorption. However, you should set the appropriate duration, depending on the application of the device.

The results we obtained can be seen in Table 2. The most interesting point is the very high extraction efficiency we obtain when the simulation size is just 1x1 period, which is 23.5%. This then falls to about 10% when the device is 3x3 periods big. That means that we should be careful with the periodic walls.

Table 2: LED extraction efficiency with a photonic crystal. This set of simulations used periodic walls and a small number of periods. Note the very high efficiency when the size of the simulation is 1x1 periods, and how it falls for bigger sizes. Also, generally the extraction efficiency increases with a longer duration. This is expected, as there was no absorption in this device. Device was LED_BigBox_SmallBox_Periodic_X-pol in sub-project "Photonic Crystal Periodic Walls".

Size (periods)	grid(um)	duration (fs)	Polarisation	Top Efficiency Small Box	Bottom Efficiency Small Box	Remaining Power
1x1	0.02	200	X	0.235	0.290	0.475
1x1	0.02	400	X	0.262	0.381	0.358
3x3	0.02	200	X	0.101	0.409	0.490
3x3	0.02	400	X	0.117	0.470	0.413
5x5	0.02	200	X	0.087	0.429	0.485
5x5	0.02	400	X	0.103	0.500	0.396
7x7	0.02	200	X	0.090	0.438	0.472
7x7	0.02	400	X	0.106	0.513	0.381

As a last set of results, we model the photonic crystal with PML boundaries. We see that the extraction efficiencies here are much smaller. That is because the size of the devices is small. Therefore the power that travels in the high index layer quickly reaches the PML walls and is absorbed, not having enough time to radiate into the air. Note that the extraction efficiency increases with increasing size, which corroborates our reasoning. Unfortunately, memory limitations did not allow us to reach the required simulation size. In fact most practical LED devices, with dimensions ~50um, will be too big to model with FDTD. A good approximation of their behavior can be obtained by using periodic walls, and setting the duration of the simulation to the time light needs to reach the edge of the device, as described previously.

Table 3: LED Extraction efficiency measured with PML walls. The disadvantage of this method is that you have to model the whole device. This may be difficult in the case of LEDs several tens of microns big, as the memory requirements can be enormous. Note that the extraction efficiency rises with increasing box size. This is because the wave that travels in the high index layer has more time to radiate into the air.

Size (periods)	grid (um)	duration (fs)	Pol.	Extraction Efficiency			
				Top BigBox	Top SmallBox	Bottom BigBox	Bottom SmallBox
15x15	0.02	200	X	0.03743	0.032888	0.149276933	0.13116084
25x25	0.02	200	X	0.054087	0.046148	0.234521225	0.20009741
35x35	0.02	200	X	0.068074	0.055543	0.295756973	0.24131257