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3D Modelling of Enhanced Surface Emission using Surface Roughening

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ABSTRACT
3D FDTD modelling is used to study the effect of surface roughening on the vertical emission of a point source emitting at $\lambda_0 = 0.94$ μm embedded in GaAs with a mirror behind the dipole. Enhancement of emission is seen at $\lambda_0 = 1.95$ μm for a rough-surface device with a perfect metal mirror placed 150 nm below the source.
Keywords: light-emitting diodes, surface roughness, FDTD modelling.

1. INTRODUCTION

Increasing the extraction efficiency of light-emitting diodes (LEDs) has been of intense interest for all spectral regions of emission. The limiting factor in the external quantum efficiency of the LED is the poor external coupling efficiency of photons out of the bulk semiconductor. This is a result of the high difference in refractive indices between the bulk semiconductor, typically $n \approx 3.5$, and the external coupling medium, often air ($n \approx 1$). Following the $\sim 1/(4n^2)$ [1] rule of thumb the external coupling efficiency in a smooth planar LED is ~2% for most semiconductor materials. Using the escape cone concept we can calculate a photon escape efficiency (discounting Fresnel reflection at the interface) via the ratio of the solid angle of the escape cone and the surface area of a sphere, see Equation (1).

$$\eta_{esc} = \frac{A_{cone}}{A_{sphere}} = \frac{2\pi r^2 (1-\cos\theta_c)}{4\pi r^2} = \frac{(1-\cos\theta_c)}{2} \tag{1}$$

For GaAs the critical angle $\theta_c = 16.5^o$; this gives an approximate escape efficiency $\eta_{esc} = 2.07\%$.

Several approaches have been identified in the attempt to increase the external efficiency of the LED. These include adding a highly reflective surface to the substrate side of the device [2, 3], applying surface roughening to the emission surface [4, 5], using novel chip geometries such as the truncated inverted pyramid (TIP) [6], the resonant cavity LED [7] and most recently using 2D photonic crystal patterns [8, 9]. This paper will concentrate on roughening as a method to increase efficiency. Most roughness models use analytical techniques [4]; however, here we adopt a 3D numerical approach using the Finite Difference Time Domain (FDTD) method. This will enable detailed study of the effects of different types of roughness and will enable accurate comparisons between different methods for increasing emission, such as those based on photonic crystals. It is also envisaged that this type of model will be ideally suited to devices that use pre-patterned roughness that is not completely random but is derived from a masking process or even direct etching using techniques such as Focused Ion Beam (FIB) etching [10].

2. FDTD MODEL

This paper will use an in-house 3D FDTD code which has been developed over a number of years and has been used extensively in the design and modelling of optical devices, in particular photonic crystal based structures [11]. In this paper an infinitesimal dipole is placed in a block of GaAs ($n = 3.48$ [12]) in the centre of a simulation space measuring 5 × 5 × 5 μm. Figure 1 shows a 3D view of the block with the roughened top surface. The block measures 5 × 5 μm in x-z plane and is 4μm thick in the y direction. A perfect metal layer is placed 150nm below the dipole in order to recycle the light scattered from the rough surface [4]. This distance is chosen to ensure constructive superposition of the electromagnetic fields from the point dipole and the virtual dipole (created by the presence of the mirror) at the surface at $\lambda_0 = 1.5$μm. Figure 2 shows a top view of the roughness pattern being used. In this case it is made up of a pseudo-random grid of 625 100 nm square air holes. The depth of the air holes is varied from 0 nm to 200 nm pseudo-randomly, while their width is roughly half an internal wavelength [4]. This type of pattern could be easily created using FIB etching. Figure 3 shows a cross section through the model at $z = 2.5$ μm. Initially the structure is meshed with ~ 2million FDTD cells, using non-uniform meshing of 25 nm ($\sim \lambda_g/11$ for $\lambda_0 = 0.94$ μm) near the dipole and 50 nm further away from the source to reduce run-time requirements. A typical run time for this structure is around 10 hours on a Pentium 4 processor. A Gaussian modulated sinewave excitation, centred at 0.94 μm is imposed on the dipole which is oriented parallel to the x-axis. The simulation is bounded on the sides and the top by 1st order absorbing boundaries after Mur [13].

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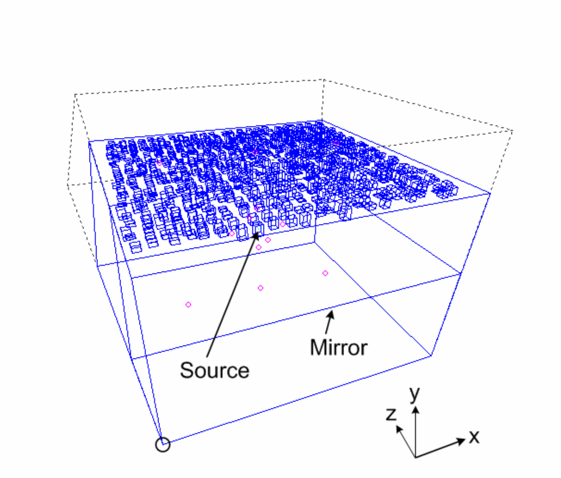

Figure 1. 3D view of FDTD model.

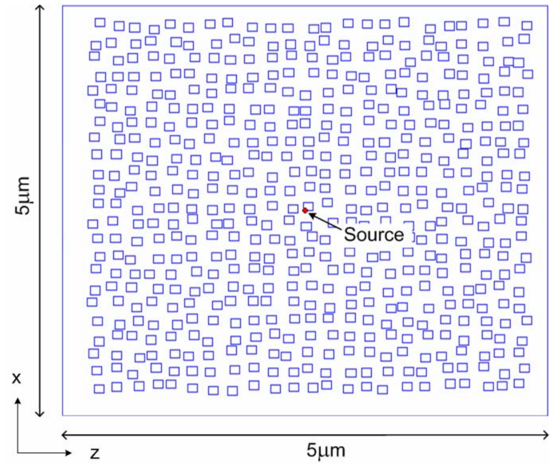

Figure 2. Top-down view of surface roughness in FDTD model (x-z plane).

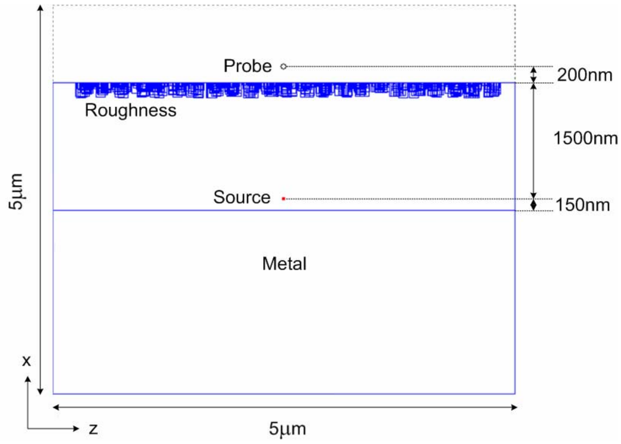

Figure 3. x-y section through FDTD model.

3. RESULTS

Models with both smooth surfaces and roughened surfaces are studied in order to be able to assess the effect of roughening the surface. These simulations are also performed with and without the mirror to show its contribution to vertical emission through the surface. Typical distributions of $|E_x|$ in the *y-z* plane at $x = 2.5$µm are shown in Fig. 4*a* and Fig. 4*b* for a smooth surface with mirror and a roughened surface with a mirror respectively. The rough surface in this case consists of 100nm square holes of random depth between 0 and 200 nm. It is difficult from these data to assess which structure is giving the strongest emission and full vertical Poynting vector calculations across the whole simulation plane at $y = 4.2$ µm for a range of wavelengths are now underway. However it is clear to see the perturbation introduced by the roughened surface.

In order to assess the wavelength dependence of the emission, single probes have been placed at regular points on the *x-z* plane above the structure at a height $y = 4.2$µm. These monitor all six field components at each time step. Thus these can be used to calculate the emission as a function wavelength using discrete Fourier transforms (FFT). Figure 5 shows the ratio in dB of $|E_x|^2$ at the centre of the block, 200 nm above the surface of the block to that for a flat block with no mirror for three different cases. Firstly, Fig. 5*a* is the case of a roughened surface with no mirror and only very slight improvement over the flat surface is seen; this to be expected, since without a mirror there is no chance to recycle the randomly reflected light into the light cone. In Fig. 5*b* data for a flat surface with a mirror added 150nm behind the dipole is shown and two features are noticeable. Firstly there is a large suppression of emission when the dipole is $\sim \lambda_g/2$ from the dipole around 1050 nm and much stronger emission when the distance from dipole to mirror is in the region of $\lambda_g/4$ (2100 nm) as might be expected, remembering that there is a π phase shift introduced by the mirror. In the case of Fig. 5*c* the roughened surface with mirror, similar behaviour is observed to that in Fig. 5*b* with suppression around

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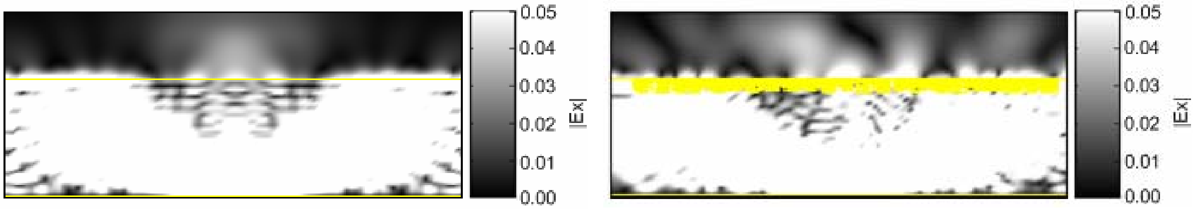
$\sim\lambda_g/2$ and enhancement around $\sim\lambda_g/4$. However, now a small region of strong enhancement exists around 1950 nm and this is most likely due to a combination of mirror and roughness recycling working together. Further investigation is required.

In order to confirm the role played by the mirror, its location is moved to 220 nm away from the source which is expected to produce strong suppression of the field at $\lambda_0 = 1.5$ µm. Figure 6 confirms that this is indeed the case.



(a) *(b)*

Figure 4. $|E_x|$ *at* λ_0 *= 940nm for (a) smooth surface with mirror; (b) roughened surface with mirror.*

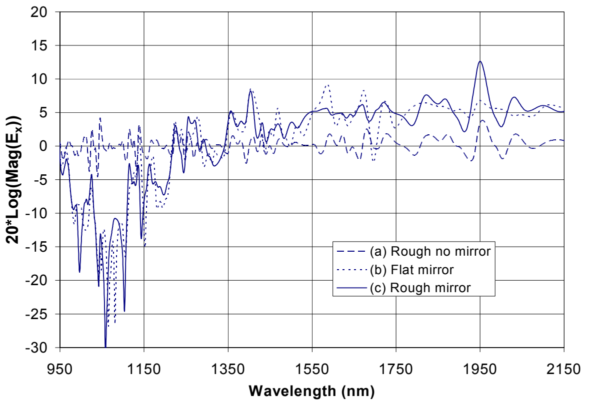


Figure 5. Ratio of (a) rough surface with no mirror, (b) flat surface with mirror, (c) rough surface with mirror to flat surface without mirror.

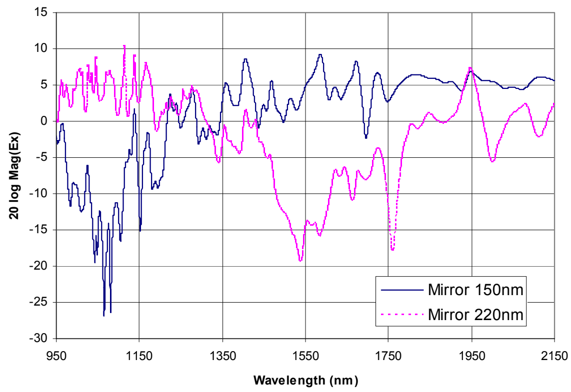


Figure 6. Data as in Fig. 6 compared for mirror locations of 150nm below source and 220nm below source.

4. CONCLUSIONS

This paper has presented results for 3D numerical modelling of emission from an infinitesimal dipole in the centre of a block of GaAs with a mirror placed 150 nm behind the dipole with and without a roughened surface. The results show that suppression and enhancement of emission is observed as expected for constructive and destructive interference caused by the mirror. A region of strong enhancement is also observed for the roughened surface where the mirror and the roughened surface work together to emit light into the escape cone. These preliminary results are for a single observation point 200 nm above the surface and detailed calculations to evaluate the total vertical radiated power and far field radiation pattern are now underway. Models investigating the effect of differing roughness depth and width and multiple sources are also planned.

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