Investigation of Nanoscale Photonic Crystal Arrays on Gallium Nitride Blue Light-emitting Diodes

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Abstract. Nanoscale photonic crystal arrays have been investigated by simulation to enhance the light extraction efficiency of blue gallium nitride light-emitting diodes. The plane wave expansion method and finite difference time domain method were used to reveal the photonic energy band gaps with the relevant structure parameters. The results showed suitable band gaps at the wavelength range of 454–606 nm for triangular lattice array with lattice constant of 200 nm. It would facilitate the design process for high-efficient diodes.

Introduction

Due to the demand of green energy technology, high-efficient gallium nitride (GaN) based light-emitting diodes (LED) have been gradually adopted as solid lighting sources [1]. However, the extraction of quantum photons is limited by the high refractive index of GaN material, which results from its own total internal reflection angle. The external quantum efficiency is relatively low. It is therefore important to investigate how to enhance the light extraction efficiency of light-emitting diodes, and the photonic crystal design provides an alternative solution [2]. As the semiconductor industry’s process technology scales can reach the nanometer level, photonic crystal technology in the range of visible light wavelength range can be achieved.

It becomes important to employ plane wave expansion (PWE) method and finite difference time domain (FDTD) method to investigate photonic crystals with relevant parameter settings, such as pattern arrangement, space parameter and dielectric constant. It is interesting to understand how photonic band gap modulation is affected by the effect of confinement, and if it can increase the efficiency of light-emitting extraction.

Photonic crystal arrays utilize periodic dielectric constant materials to manipulate photon pathway [3, 4]. A portion of the wavelength in the assignable direction can form a confined effect. It has been suggested that the increase in light extraction efficiency may come from three different mechanisms. First of all, it is prevention of lateral propagation of light and enhancement in the vertical direction. Also, the photonic crystals can act like Bragg grating structure and produce multiple diffraction effect. The photon thus has more chance to escape out of the device. Finally, the multiple diffused scattering of light breaks the total internal reflection angle and then enhance the light extraction efficiency.

In this study, two-dimensional photonic crystal analysis by simulation has been carried out for the light intensity, compared with those different parameters. In addition, the control of air hole depth in the slab involves another dimension to be discussed. The investigation utilized the plane wave expansion method and the finite difference time domain method for photonic crystal arrays on blue GaN light-emitting diodes with the emitting wavelength of 463 nm. The results can be further applied in the design process.

Experimental Details

The simulation process involves Bloch’s theorem and Maxwell’s eqs. The theorem simplifies the complexity of wave propagation. It is periodic and we can make use of Brillouin zone to assist the
analysis of energy band. Electromagnetic waves can be expressed, with potential periodic
distribution, by Fourier series expansion:

\[
\begin{align*}
\vec{H}(\vec{r}) &= \sum_{\sigma} \vec{H}_\sigma(\vec{G})e^{i(\vec{G}+\vec{k})\cdot \vec{r}} \\
\vec{E}(\vec{r}) &= \sum_{\sigma} \vec{E}_\sigma(\vec{G})e^{i(\vec{G}+\vec{k})\cdot \vec{r}}
\end{align*}
\]

and the master equation:

\[
\begin{align*}
\frac{1}{\varepsilon(r)} \nabla \times \left( \frac{1}{\varepsilon(r)} \nabla \times E(r) \right) &= \frac{\omega^2}{c^2} E(r) \\
\nabla \times \left( \frac{1}{\varepsilon(r)} \nabla \times H(r) \right) &= \left( \frac{\omega}{c} \right)^2 H(r)
\end{align*}
\]

where, \( \varepsilon(r) \) is the dielectric constant, \( \omega \) is the angular frequency of light, and \( c \) is the speed of light.

We can get

\[
\begin{align*}
-\sum_{G'} K(G-G')(k+G') \cdot (k+G') E(G') &= \frac{\omega^2}{c^2} E(G) \\
-\sum_{G'} K(G-G')(k+G') \cdot (k+G') H(G') &= \frac{\omega^2}{c^2} H(G)
\end{align*}
\]

A series of changes in the values of wave vector \( k \) can be obtained by a series of characteristic frequency \( \omega \) with these solutions. The expression is plane wave expansion method, as well as the concept of calculus to position the energy gap’s principle to build energy-band structure [5]. The order of the photonic crystal array has the most direct impact on the Brillouin zone, either triangle or cubic in the array (Fig. 1). The corresponding Brillouin zones are shown with symmetry. It is noted that the choice of triangular array model provides more band gaps [6].

![Figure 1. Triangular array and cubic array with the respective Brillouin zones](image)

**Results and Discussion**

The enhancement in light extraction efficiency may include two mechanisms, suitable photon energy gaps and surface roughness effect that generates diffusing light. At first, we modulate the triangular photonic crystal lattice constant (200~800 nm) with holes in slab. The air hole radius was
fixed at 75 nm. The results showed photon energy gaps for only 200 nm and 300 nm lattice constants. The gaps existed at the wavelength range of 454–606 nm for 200 nm lattice constant (Fig. 2), and 967–1071 nm for 300 nm lattice constant. Larger lattice constant sample showed no band gap (Fig. 3). The emitting light wavelength was set at 463 nm.

The design parameters have been studied with different radius of 60 nm, 75 nm and 80 nm. With the FDTD FullWAVE simulation process, it is also interesting to change the depth of holes to test the extraction efficiency. At 50 nm depth, the time-domain light intensity is shown in Fig. 4. Even with the photon energy gap, the time-domain change in light intensity and spatial light intensity can be seen in comparison to the performance parameters of the more prominent group of 800 nm. In two-dimensional photonic crystal with air holes, the interesting phenomenon is observed in some specific geometric arrangement [7]. The conformation diffused into the effect of scattering light.

The results for a higher depth of 200 nm are displayed in Fig. 5 and Fig. 6. The results from the simulation are indeed as previously assumed, inside the conduction mode by the means of photonic
band gap to the radiation modes [8]. The results indicated that light-emitting intensity could
enhance the space outside the light intensity. This phenomenon is the limitation of photonic band
gap effect. The depth must comply with the appropriate parameters. During an actual manufacturing
process, it may be caused by the non-convergence coupling effect of ratio, or the status of a number
of surface states for the extraction effect. It is always possible to have a scattering effect at the same
time with the photonic band gap effect. The parameters must be carefully designed.

Conclusions

In summary, the best photonic band gap limitation has been found for the triangular lattice array
with the lattice constant of 200 nm, and the production of air holes for a radius of 75 nm. When the
lattice components in the triangular array of circular holes were supplemented by close to the depth
of 200 nm in the GaN layer, the external light field intensity could be enhanced up to about 90%. In
addition, the data structure in the theoretical deduction included simple assumption, and the
manufacturing process is more difficult for follow. It may be optimized for the light extraction
effect to be improved. On the other hand, it is always possible to have a scattering effect at the same
time with the photonic band gap effect. The photonic crystal parameters need be carefully designed
accordingly.

![Figure 5. Comparison of spatial light intensity, at 200 nm depth.](image)

![Figure 6. Time-domain light intensity, at depth of 200 nm.](image)
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