Simulation and Experiment on 2PC Transmitted Diffraction Grating for GaN LEDs

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ABSTRACT

To test 2PC structures by experiment, we affixed 2PC structures onto a hemicylinder of polydimethylsiloxane (PDMS) and placed the sample on a rotating stage with a green laser beam (λ=532nm) incident on the grating structure. Besides the experimental tests, theoretical models are developed to predict experimental results. The source for the finite difference time domain (FDTD) simulation was a plane wave with a Gaussian power distribution. Comparing the simulation results with the experimental ones, we found that FDTD underestimates the experimental data and does not account well for the upward inflection of transmission efficiency about the critical angle. To increase the accuracy, a more finely girded simulation at the diffraction grating is developed, and this result agrees very well with the experimental test.

1. Introduction

The focus of this particular research project is on developing higher brightness, higher efficiency and longer lifetime of GaN-based light emitting diodes (LED), an important research topic in solid-state lighting, the so called next generation lighting.

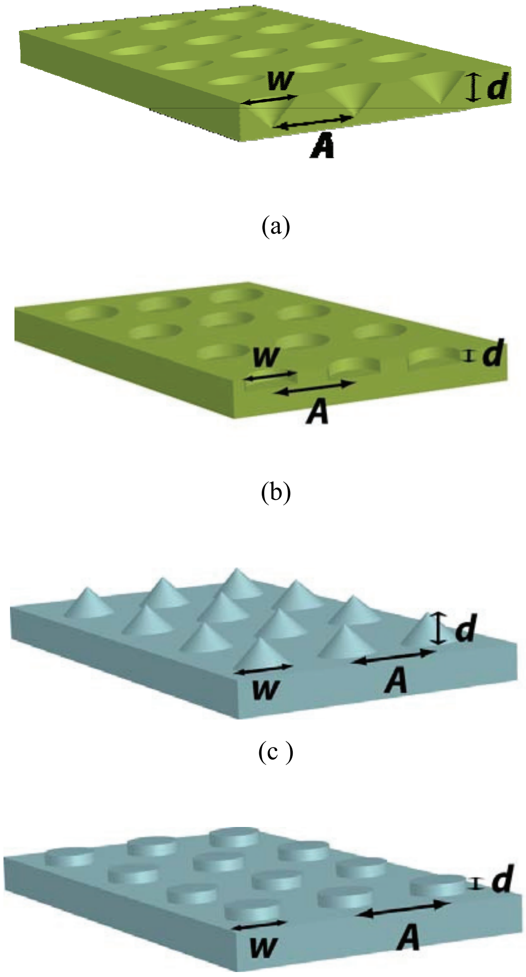
Problems to be addressed: The current advancements allow us to achieve applications with LEDs in fiber optics, displays, and lighting systems. We can even control the color contrast of the device and create a full color set with red, green, and blue LEDs [1]. Although LEDs have been used in many applications, the light extraction efficiency is still very low for Gallium-Nitride (GaN) LEDs due to several factors: GaN has a low critical angle that traps light inside the device [2], absorption of light within the device due to dislocations and defects within the GaN crystal [3], and a device design and structure that has not been optimized (ie. epitaxial side up vs. epitaxial side down chip structures) [4]. It is critical to develop LED technology to reduce energy consumption through higher efficiency of LEDs and expedite resulting replacement of older, less efficient technologies.

The greatest limitation in GaN-based LEDs is the effect of total internal reflection resulting in poor light extraction efficiency (LEE). This applies to any large change in refractive index on the boundary between two materials. When light is above the critical angle, the light cannot escape and is eventually absorbed in the device, decreasing LEE and generating heat. Many methods of improving LED efficiency are currently being explored. Almost all of these methods are seeking to extract the trapped light in greater quantity and faster speed. Those methods being explored are placing photonic crystals or a nanostructure grating on one of LED layers to modify the effective index of refraction at the boundary [6-7], randomized roughening on the surface of the device [7-8], slanted device configurations that result in pyramidal shapes [7], and inverted “flip-chip” designs that put the epitaxial side upwards or downwards [4] [9].

2. Simulation Model

The research goals: (1) simulate 3-D structures that do not approximate LED chip surfaces to two-dimensional structures, as in two-fold photonic crystal (2PC) structures, (2) accurately simulate such a 3-D grating structure, (3) produce simplifications to such a model to increase stability and reduce simulation time, and (4) collaborate and synergistically work towards developing experiments and fabrication processes to compare with 3-D simulations.

Because of the stated issues of light extraction due to GaN’s low critical angle, a key component of our research was to solve the light trapping issue by a common solution: etch a periodic structure on one or more of the GaN layers to allow transmitted diffraction to allow light to escape for angles past the critical angle [12]. Various grating structures exist, such as hemispheres, cylinders, pyramids, cones, and other arbitrary shapes. All structures can be in hole or pillar formations. The most common structures are conical and cylindrical, due to the ease of fabrication. Fig. 1 shows the possible grating structures for the conical and cylindrical shapes. Study of these grating structures involved two parts: the study of transmitted diffraction from 2PC structures and also the study of top transmission gratings on LED devices, both of which are reported on in the following sections.



(a)

(b)

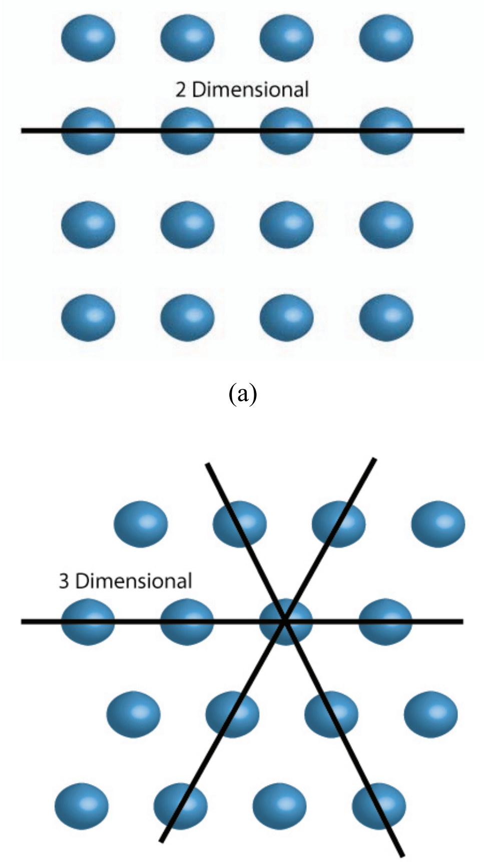
(c)

(d)

Fig. 1 - 2PC Grating Structures: (a) conical holes, (b) cylindrical holes, (c) conical pillars, and (d) cylindrical pillars

3. Experimental Setup

2PC Transmitted Diffraction: To test these structures by experiment, we affixed 2PC structures onto a hemicylinder of polydimethylsiloxane (PDMS) and placed the sample on a rotating stage with a green laser beam (λ=532nm) incident on the grating structure. The 2PC hole arrays had a lattice pitch of 2μm and were prepared on a silicon wafer with an area of 1mm×1mm. The 2PC pattern was then transferred onto the planar center point of the PDMS hemicylinder by soft nanoimprinting. [10,11] A photodetector was placed behind the grating structure to measure transmission efficiency. Since we were interested only in single-pass transmission characteristics, the hemicylinder shape allows reflected and diffracted light to escape with negligible reflection back towards the photodetector. Fig. 3 shows the experimental model and grating structure.

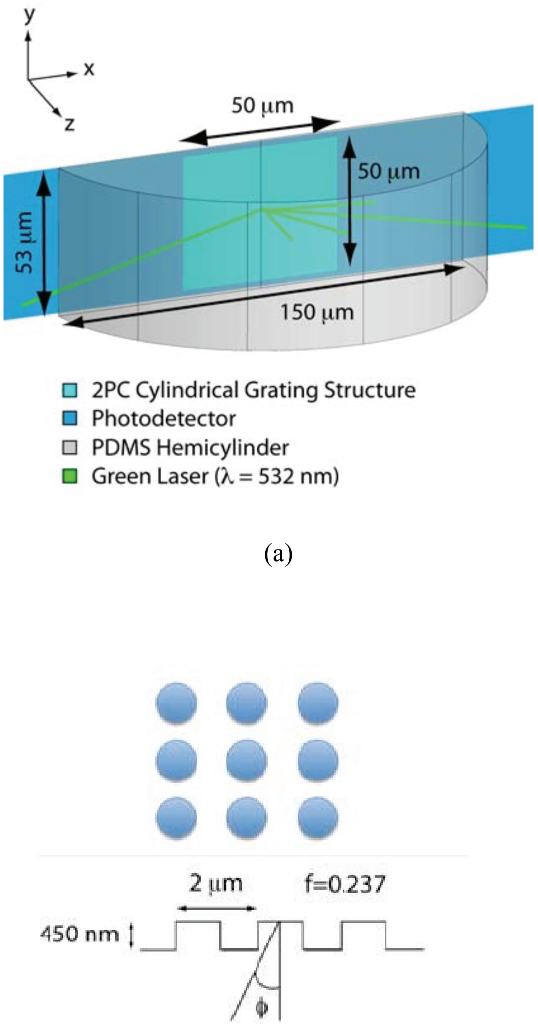


(a)

(b)

Fig. 2 – Grating structures of various dimensionality: (a) 2-D approximation of a 2PC grating structure and (b) a full 3-D model of a 3PC grating structure

(d)



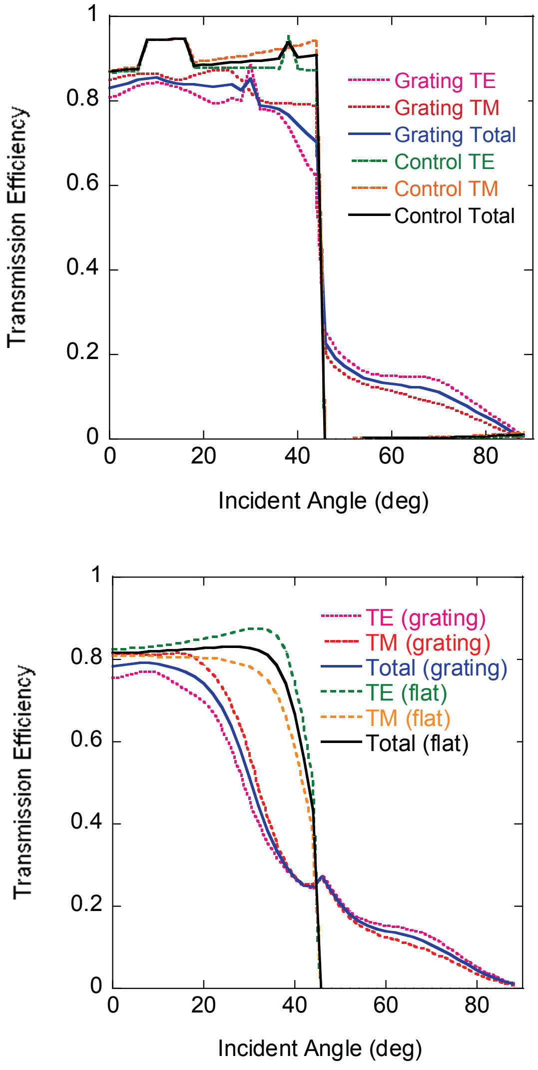
(a)

(b)

Fig. 3 – Experimental setup for measuring transmitted diffraction of a 2PC structure mounted on PDMS

4. Results

Also, we used theoretical models to predict experimental results. Since the symmetry is 2-fold, this allows us to use 2-D models to represent an otherwise 3-D model. 2-D models bear heavy costs in simulation time and required memory in FDTD. These requirements are somewhat more relaxed in Rigorous Coupled Wave Analysis (RCWA). [10,11] Fig. 4(a) shows a 2PC structure that can be simulated as a 2-D model, while the three-fold symmetric photonic crystal structure Fig. 4(b) cannot be approximated by 2-D models, due to the honeycomb pattern whose diffraction effects cannot be approximated, as is the case with 2-D simulation models. The results of the simulations in FDTD and RCWA are shown in Fig. 4a and Fig. 4b, respectively. Simulations by FDTD using a Yee's mesh were coarsely gridded at a Δx of 200nm and a Δz of 45nm. The source for the FDTD simulation was a plane wave with a Gaussian power distribution. The simulation domain included 100 grating cells at a lattice pitch of 2μm, filling factor of 0.237, and grating cell height of 450nm. RCWA simulations assumed an infinite plane of grating cells with a rectangular plane wave source are also performed for comparison.



(a)

Fig. 4 (a) Transmitted Diffraction Efficiency simulatin by FDTD simulation and (b)Transmitted Diffraction Efficiency for a non-uniform gridded FDTD simulation.

The results of the simulations show that RCWA produces a more accurate model of the experimental data. FDTD underestimates the experimental data more than RCWA and does not account well for the upward inflection of transmission efficiency about the critical angle. To increase accuracy, a more finely gridded simulation is necessary. When using FDTD, a method to gain higher resolution at critical points, such as a diffraction grating, while still keeping a coarse grid for the rest of the simulation domain is to use a non-uniform grid. This allows simulation time and memory to be kept low while not sacrificing accuracy at critical points in the diffraction grating as shown in Fig. 4. The simulation only uses a non-uniform grid in the z-direction. The smoothness of the simulation data for both grating and flat cases is accounted for by the fine grid at the grating (Δz = 22.5nm), while the simulation time was kept low by making the rest of the simulation area coarsely gridded (Δz = 56.25nm). The inflection is now clear at an incident angle of 46 degrees but is still not as accurate as the RCWA simulation model. This is a definite disadvantage of FDTD, in that transmission properties are not easily measured, as material dispersion, near field effects, coarse/fine gridding can affect the accuracy of an FDTD model. For regular structures, methods such as RCWA are more efficient and more accurate for calculating transmitted diffraction.

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