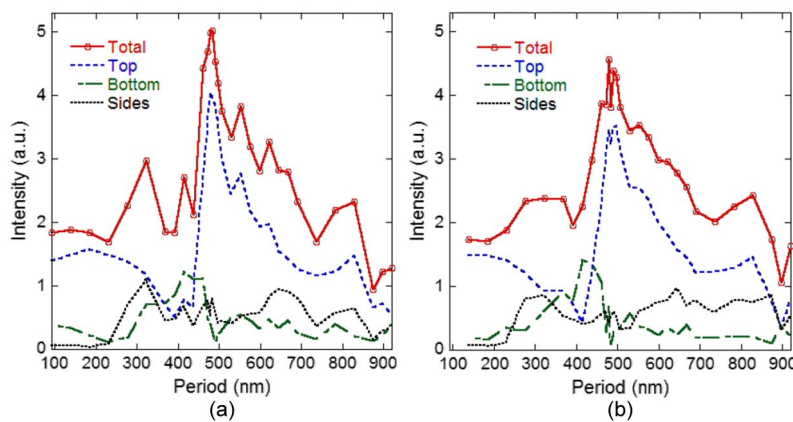
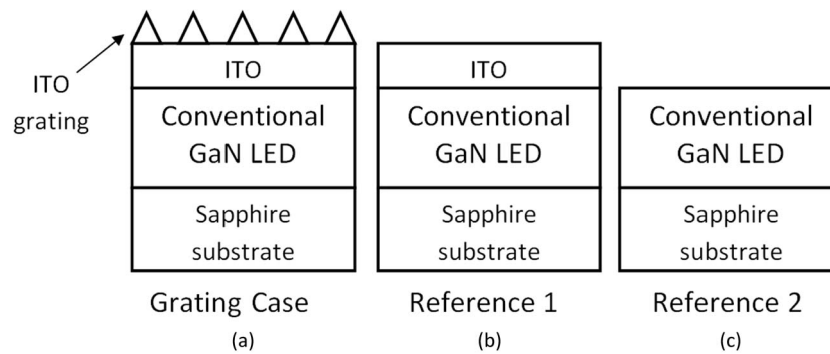


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Abstract: This study reveals the effect of nanoscale ITO transmission gratings on light emission from the top, sides, and bottom of a GaN light-emitting diode (LED), based on the substrate standing wave analysis. First, we show that sapphire substrate thickness affects the standing wave pattern in the LED and find the best- and worst-case sapphire thicknesses. Second, we find that adding nanoscale ITO transmission gratings can improve light extraction by 222% or 253%, depending on the reference chosen. Third, we observe that maximizing top light emission with the nano-grating can significantly reduce bottom and side light emissions. Finally, we study grating performance over different wavelengths and generate the LED spectrum.

Index Terms: Grating, nano-scale, LED, GaN.

1. Introduction

Over the last 60 years, annual electricity consumption in the U.S. has increased by 1300% to 3856 terawatt hours. Lighting, at 17% of all US residential and commercial electrical use, stands out as a significant area to reduce energy consumption [1]. While the reasons to reduce energy use vary from government objectives such as achieving energy independence to corporations' seeking larger profit margins and reducing environmental footprints. In general, reducing the consumption of electricity through more efficient lighting is desired. A report [1] from the U.S. Office of Energy Efficiency and Renewable Energy projects that switching to light emitting diode (LED) lighting over the next 20 years will save 46% of electricity used in lighting. Gallium nitride (GaN) LEDs are an important component in this progressing to solid state lighting since they are the most potential blue/green light sources currently.

In general, the efficiency of a GaN LED is limited by the maximum angle that light can escape from the surface as defined by Snell's law [2]. Since GaN has a high index of refraction compared to air, light can only escape from the LED if it approaches the surface within 23° of normal. Adding a material with an index of refraction between the indices of GaN and air to the LED surface increases the limiting angle [3]–[7]. Creating sub-wavelength nanostructures at the LED surface can also increase the limiting angle by having a graded index of refraction between GaN and air that has

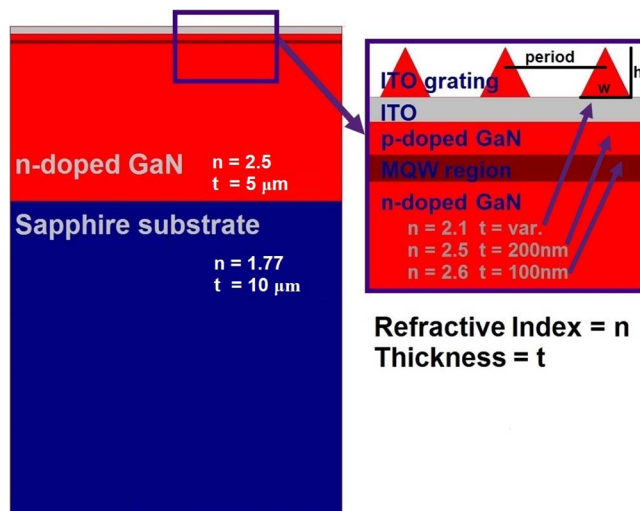


Fig. 1. Simulation model of LED used in the FDTD calculations.

anti-reflection properties [8]. Gratings increase light output by providing additional angles for light to escape and by breaking up lossy waveguide modes within the LED. Recently several research groups have placed gratings either on the surface [3], [4], bottom [3], or sides [8] of the LED. However, most publications on transmission gratings are either focused on micro-grating simulation [3] or are experiments in the micro-grating [4]–[9], [4]–[14] or nano-grating [18]–[20], [23], [24] ranges. In their research, the types of gratings vary: some researchers use uniform geometrical patterns [6], [7], [19]–[24], while others use randomly placed geometrical surface features [14], [19], [22]. In a third and simpler approach, researchers roughen the LED surface to increase the number of angles that light can strike the surface [16]–[18]. The above studies focused exclusively on grating efficiency instead of other important factors.

Light extraction location in GaN LEDs was studied in 2005 [25], while cavity mode research was presented in 2011 [26] and 2013 [27]. In this paper, we investigate why adding nano-gratings improves LED light extraction efficiency by simulating the internal electromagnetic (EM) field inside the LED cavity and find the standing wave pattern. We clearly show how LED efficiency is affected by the internal electromagnetic field distribution; in here is the standing wave pattern.

In general, comprehensive study on ITO nano-gratings with standing wave analysis is still very novel in this field. We provide a systematic study of nanoscale transmission ITO gratings, considering standing wave effects through the finite difference time domain method (FDTD) simulation. And we find the following novel statements: First, adding a thin ITO layer can provide the highest average light output while minimizing output fluctuation when sapphire substrate thickness varies. Second, implementing a nano-scale cone grating at an optimal period, appropriate ITO thickness, and sapphire thicknesses can substantially increase light output. Third, optimizing the LEDs optical properties at the primary wavelength significantly increases the light output across the entire LED emission spectrum.

2. Simulation Model

We use the finite difference time domain method to analyze the GaN LED. FDTD is derived from Maxwell's equations and can accurately simulate the nano-grating influences in LEDs, such as reflection due to linear dispersion or total internal reflection, transmission of escaping light from the LED, and scattering at the grating. Since FDTD decomposes space and time into separate components, the model is meshed into small square cells. To obtain reliable results, the cell length should be much smaller than the wavelength of light being analyzed. The LED model, shown in Fig. 1, is developed based on Peking University experiments [3], [4]. It consists of an ITO top

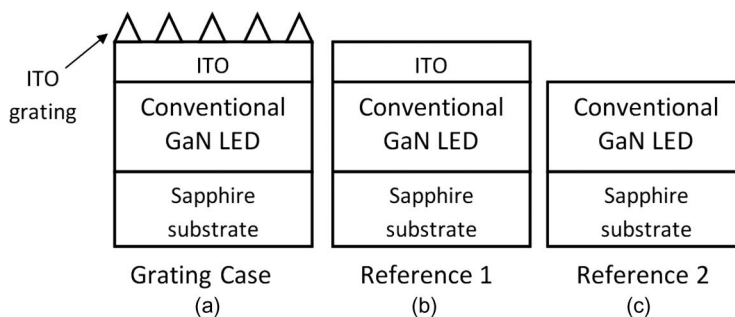


Fig. 2. LED model with (a) Grating case, (b) Reference 1, none grating, and (c) Reference 2, conventional.

grating, ITO layer, p-doped GaN, multiple quantum well region (MQW), n-doped GaN, and sapphire substrate. As shown in Fig. 2, we compare the ITO nano-grating LEDs to LEDs without gratings (reference 1), and to a conventional LED (reference 2). In most experiments and applications, light is normally collected from the top of the LED; however, we include the side and bottom light emissions in this study because they influence top emission and reveal the light distribution within the LED. The ITO grating is made from cones of equal height and width implemented with a fill factor of 0.5. The parameters, such as height and width, are important and examined more closely in our other studies [3], [20], [29], and we fixed those parameters throughout this paper to focus on standing wave field distributions and grating period study. The grating period is kept within current fabrication capabilities and ranges from 92 nm to 920 nm.

In our model, light sources are inserted into the model as a continuous, plane wave source emitting from the middle of the MQW region. The LED is surrounded by the air. The perfectly absorbing light monitors are used to measure the electromagnetic field intensity emitted into the air. The bottom and the side monitors are placed 100 nm from the LED surface while the top monitor locates 100 nm above the top of the grating (470 nm above the non-grating LED surface according to Fig. 2). The domain calculated by the computer includes the LED and the air between the LED and light monitors.

3. Simulation Results

3.1. Standing Waves

First, we study the effect of varying sapphire substrate thickness on light emission of LEDs. A standing wave exists in the LED above the MQW region and ITO thickness affects the portion of the standing wave pattern above the MQW region as shown in our previous paper [23]. However, Ref. [23] only considers top light emission. In this paper, we also present the light emitted from the sides and the bottom, and find that they clearly influence the top light emission. Based on Ref. [23], we need to consider three different ITO cases according to Fig. 2(b): a best-case ITO thickness of 78 nm, a worst-case ITO thickness of 260 nm, and a thin ITO layer of 46 nm. Fig. 3 shows that increasing sapphire substrate thickness modifies the standing wave pattern at those three ITO thicknesses.

In general, top light emission is preferred over bottom or side light emission. Fig. 3 shows that our LED emits most of its light from the top, while the sides emit the least light. It also shows that modifying the ITO and sapphire substrate thicknesses can selectively increase the top light emission while simultaneously reducing side and bottom light emission. However, total light emission is minimized when top light emission reaches its peak value because bottom and side light emissions approach zero at that point. It is very interesting that total light emission reaches its maximum output at the top light emission minima, the bottom emission maximum, and side light emission maximum. In general, light emission is best utilized when it emits from the top of the LED, we better design the LED to maximize top light emission.

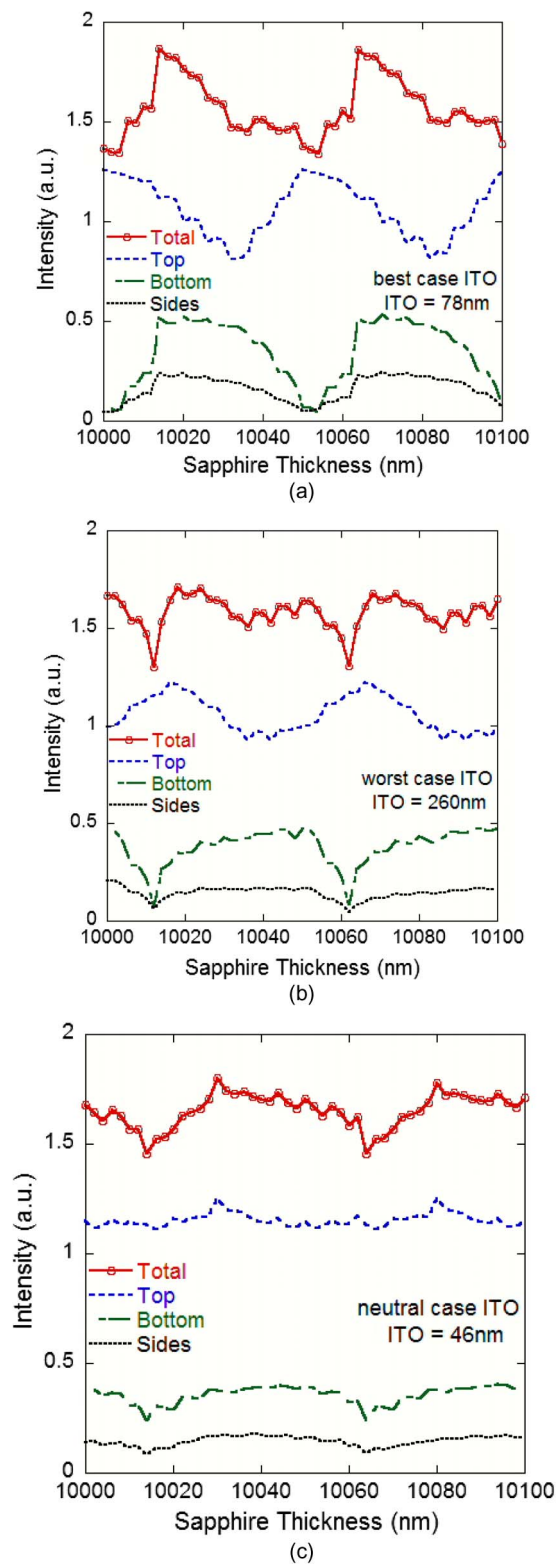


Fig. 3. Light intensity output as sapphire substrate thickness is varied with (a) a best-case ITO thickness, 78 nm, (b) a worst-case ITO thickness, 260 nm, and (c) a neutral ITO case, 46 nm.

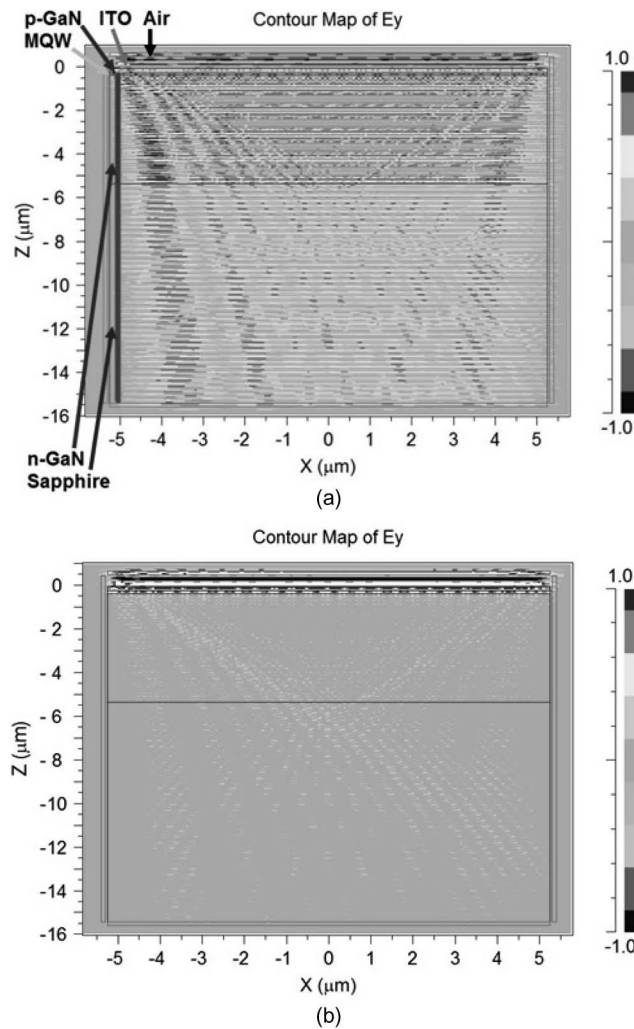


Fig. 4. Electromagnetic fields in the LED with ITO thickness 78 nm and Sapphire thickness is (a) $10.032 \mu\text{m}$, the worst standing wave condition; and (b) $10.050 \mu\text{m}$, the best standing wave condition.

Fig. 3(a) shows that increasing the sapphire substrate can reduce the best-case ITO top light extraction from 1.26 a.u. to 0.81 a.u. From Fig. 3(b) we observe that increasing the sapphire substrate increases the worst-case top light output from 0.92 a.u. to 1.22 a.u. To better explain our data, we study the electromagnetic field distribution in our LED. These results show that varying sapphire layer thickness in the LED changes the standing wave conditions. Fig. 4(a) shows that the worst-case thickness causes the light to strongly propagate through the n-GaN and sapphire substrate in the interference pattern. The best-case thickness causes the standing waves in Fig. 4(b) to have strong constructive interference at the ITO to air interface. When the EM waves in the n-GaN and sapphire layers have a destructively interference, the EM field is completely weakened.

In the thin ITO case, Fig. 3(c), we observe significantly less variation in light output. While its maximum top output approaches the best-case maximum output, its worst output of 1.11 a.u. is significantly better than the worst output of the other two cases. Also, its average top light output of 1.15 a.u. is much better than the average output of 1.06 a.u. for the other two cases. This shows that the thin ITO layer removes most of the standing wave variation while significantly increasing the average light output from the LED. Our simulations show that the substrate thickness has significant effects (ignoring fabrication limitations) and that selecting the right ITO thickness can substantially remove the effects of substrate variation and increase average light output across the LED.

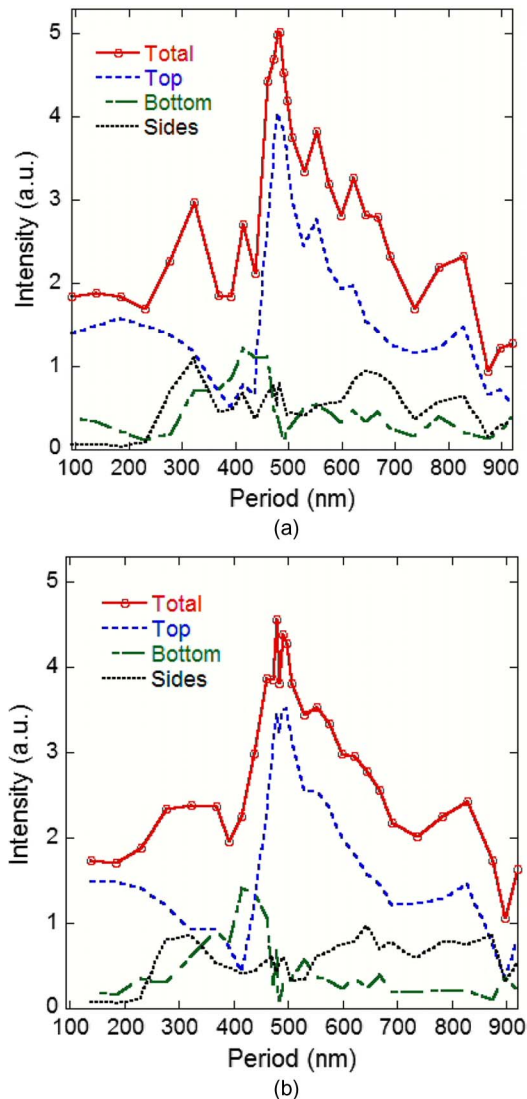


Fig. 5. Light extracted from LED as grating period is varied using (a) a best-case standing wave pattern of ITO thickness 78 nm and sapphire thickness 10.050 μm and (b) a worst-case standing wave pattern ITO thickness 260nm and sapphire thickness 10.000 μm .

3.2. Nanoscale Gratings

The nano-gratings are simulated within the current range of fabrication parameters and period varies from 92 nm to 920 nm. According to our pervious publications (Ref. [23] Ref. [29]) which provide nano-grating height and fill-factor effects, we choose our nano-grating with 50% fill factor in this paper. The ITO thickness of 78 nm and sapphire substrate thickness of 10.050 μm in Fig. 5(a) are also used because standing wave analysis demonstrates that they give the highest top light extraction, 1.26 a.u., of all cases. For comparison, the worst-case standing wave conditions found in Ref. [23] (ITO thickness 260 nm and sapphire substrate thickness 10 μm) are used in Fig. 5(b). Fig. 5 shows that the grating can decrease or increase top light emission from the LED. However, at a period of 478 nm, the grating dramatically increases both top and total light extraction while decreasing bottom light emission. The maximum top light extraction in Fig. 5(a) increases to 4.056 a.u., a 253% improvement over the conventional LED's 1.150 a.u. top output and a 222% improvement over the best standing wave output of 1.260 a.u. At peak output the grating not only increases top light

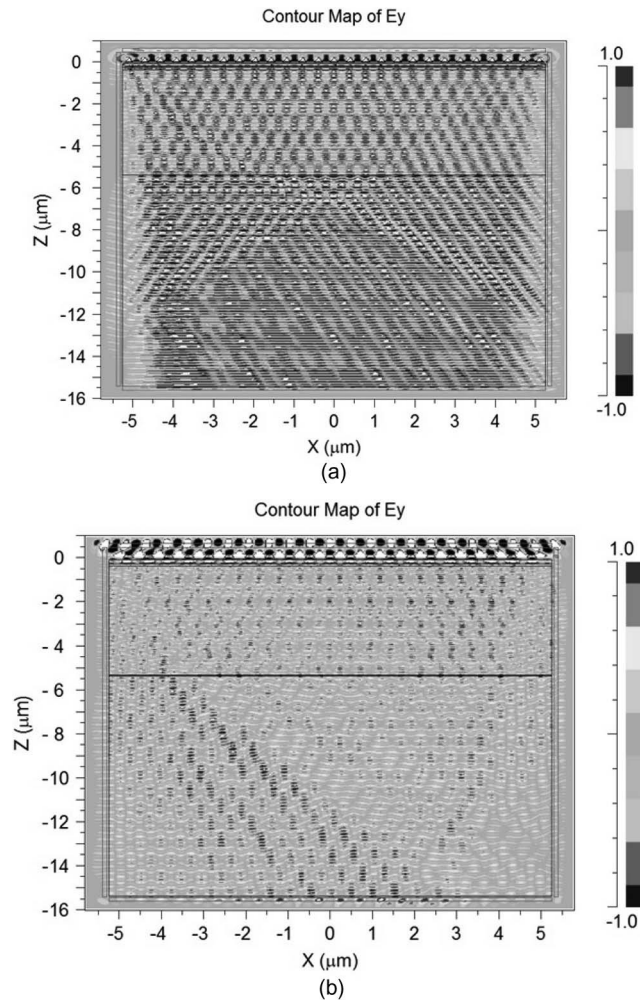


Fig. 6. Electromagnetic fields in the LED with grating periods of (a) 388 nm, the worst top light extraction and (b) 478 nm, the best top light extraction. Both diagrams have ITO thickness 78 nm and sapphire thickness 10.050 μm .

emission, but also causes 81% of all light emitted from the LED to exit from the top. This preferential light output shows that the device can efficiently direct light and operate at much higher light extraction efficiency when using a grating period of 478 nm. This is because the standing wave pattern created by the sapphire layer interacts with the interference patterns generated by the nano-grating. When the grating gives the worst top light output at a period of 322 nm, the standing wave pattern in the LED creates a strong constructive interference in the sapphire substrate and only very weak EM fields can exist at the top of the LED, as shown in Fig. 6(a). But, when the best grating period is used, 478 nm, the EM fields in Fig. 6(b) show that the light is extremely concentrated in and above the grating, while very little constructive interference occurs in the n-GaN or sapphire layers. For comparison, when a LED with an ITO thickness that provides a worst-case standing wave condition is simulated with nano-gratings, Fig. 5(b), the output intensity curve is similar to, but significantly lower than that in Fig. 5(a). Its maximum top light output of 3.518 a.u. is 14.2% lower than the 4.056 a.u., the maximum output when the best-case thicknesses are used.

By appropriately designing material thicknesses and the grating period, top and total light extraction from the LED can be greatly enhanced, while the bottom and side emissions are reduced. This greatly improves device efficiency. Therefore, implementing nano-gratings is worth the additional fabrication time and cost of implementation.

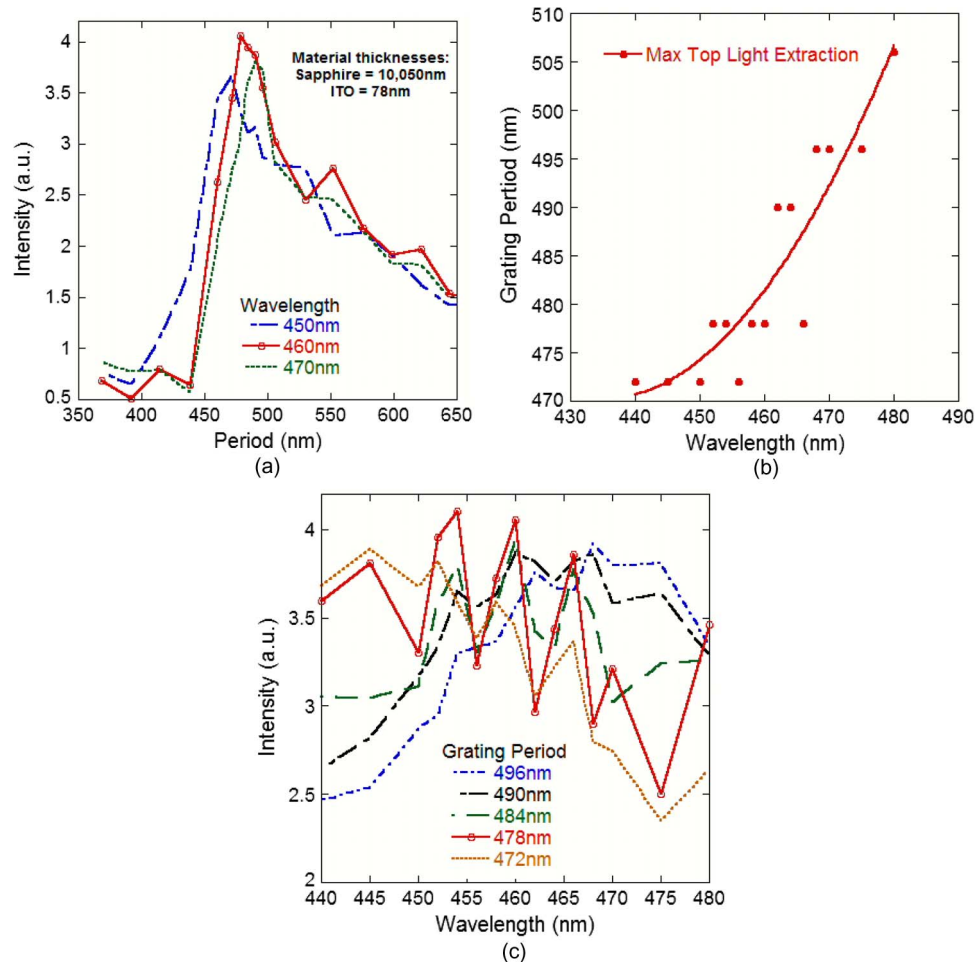


Fig. 7. (a) Light extraction at three different wavelengths. (b) Grating period for maximum light extraction vs. wavelength. (c) Light extraction intensity across the LED emitting spectrum.

3.3. Wavelength Dependent Grating Performance

LEDs emit light over a range of wavelengths, not just at the center wavelength. For the grating to be effective, it must enhance light extraction across the entire LED emitting spectrum. Fig. 7(a) compares the light extraction of 450, 460, and 470 nm and shows that they experience similar improvements in light extraction efficiency. However, the maximum power output for each wavelength occurs at a different grating period. Fig. 7(b) shows that for maximum top light extraction, shorter wavelengths correlate with smaller grating periods and longer wavelengths correlate with bigger grating periods. Because the material layers are optimized for 460 nm light in the standing wave section, as the wavelength increases or decreases from 460 nm, the standing wave conditions will first cause destructive interference at the LED surface, then cycle back to constructive interference again. In Fig. 7(c), this effect is very pronounced with the 478 nm grating period that maximizes light extraction at the center wavelength, 460 nm. In Fig. 7(c), we also show that larger grating periods like 496 nm enhance the longer wavelengths of light within the LED emitting spectrum and shorter periods around 472 nm enhance the shorter wavelengths, which is also shown in Fig. 7(b) as well. Since the most LED light is emitted around the center wavelength, the grating period that maximizes total light output for our design is a grating period near 484 nm. The results in Fig. 7 are expected due to the general physics of sub-wavelength grating where optimum spectrum is obtained for period beneath the incident wavelength. Currently sub-wavelength gratings are still a

fairly active field of research. The most obvious effect of sub-wavelength gratings is strong polarization, but our simulations are only focused on total field distributions and do not consider each polarization separately.

4. Conclusion

Standing wave analysis of the LED shows that light extraction efficiency is affected by both ITO and sapphire substrate thicknesses. These two parameters can cause top light output to range from 0.809 to 1.260 a.u., which is about 56% variation. Adding an ITO cone grating of period 478 nm to the best standing wave case can substantially increase both top and total light output while decreasing output from the bottom and sides. The grating's top light output is 4.056 a.u., 222% better than the best standing wave top output and 253% better than the conventional LEDs top output. Designing nano-scale ITO gratings, ITO thickness, and sapphire thicknesses can substantially improve LED light emission by increasing light output both at the center wavelength and across the emission spectrum.

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