Design of out-coupling structures with metal-dielectric surface relief

Sun-Kyung Kim, Ho-Seok Ee, Kyung-Deok Song, and Hong-Gyu Park*

Department of Physics, Korea University, Seoul 136-701, South Korea
*hgpark@korea.ac.kr

Abstract: We propose an unconventional out-coupling structure consisting of two-dimensional periodic metal-dielectric patterns. Numerical simulations show that low orders of guided modes are extracted efficiently by the metal-dielectric pattern with a pitch size of ~(λ/n) and pattern depth of <100 nm. Vertical GaN light-emitting diodes with optimized metal-ITO patterns exhibited extraction efficiencies enhanced by factors of 6.6 and 2.6 for perfect conductor and silver metals, respectively, as compared to a non-patterned structure. The plasmonic absorption loss from the corrugated silver mirror accounts for the relatively smaller enhancement in extraction efficiency with the silver-ITO pattern. Furthermore, a double-sided out-coupling structure consisting of an upper GaN-air pattern and a bottom perfect conductor-ITO pattern exhibited a 40% enhancement in extraction efficiency as compared to the structure with single GaN-air pattern. We believe that deep understandings of the interaction between light and metal-dielectric patterns will lead to improved device performances in various optoelectronic applications including high-efficiency light-emitting diodes.

OCIS codes: (240.6680) Surface plasmons; (230.3670) Light-emitting diodes; (050.0050) Diffraction and gratings.

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1. Introduction

Semiconductor light-emitting diodes (LEDs) show unique advantages such as easy integration with other optical components, high color rendering index, and long device life time. Although incandescent or fluorescent classical light sources still occupy a major portion of the present market, LEDs will become dominant in the market for general illumination if the efficiency of LEDs increases further [1]. In general, to improve the efficiency of LEDs, one can consider the following three methods: the enhancement of internal quantum efficiency through abrupt defect-free epitaxial growth, the enhancement of out-coupling efficiency through an appropriate chip design, and the design of packages including a phosphor with high conversion efficiency. In particular, regarding the improvement of out-coupling efficiency, several ideas have been proposed such as surface roughening [2–4], periodic patterning [5–8], and resonant cavity effects [9–11]. However, no other approaches have surpassed the conventional surface roughening technique in terms of light extraction efficiency [12].

A GaN blue-emitting LED is an essential component in white light sources using down-conversion phosphors. Recently, laser or chemical lift-off GaN vertical LEDs have become crucial for high-output applications such as general illumination and backlight units for large-area displays because of its efficient thermal dissipation and uniform current flow [6,8,13–15]. In this paper, we propose a GaN vertical LED with a two-dimensional (2D) periodic metal-dielectric pattern as an efficient out-coupling structure. Using numerical simulations, we illustrate extraction mechanisms and design rules of the metal-dielectric patterns that distinguish them from conventional dielectric out-coupling patterns.

2. Design rules of out-coupling patterns on a dielectric slab

Figure 1(a) shows the schematic of the vertical GaN LED structure with a top dielectric periodic pattern and a bottom metal mirror. When photons are generated inside the GaN slab, some photons are trapped in the slab and coupled to guided modes. To extract these trapped photons, an appropriate out-coupling structure that perturbs the evanescent tail of guided modes is incorporated into the GaN slab. Therefore, it is useful to calculate a modal index for each guided mode, which is defined by the propagation constant of the mode divided by the

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vacuum wavenumber, as a way to qualitatively understand how the out-coupling structure interacts with the guided modes. Figure 1(b) shows the calculated modal index for several guided modes as a function of the thickness of GaN slab using a beam propagation method (BPM). The BPM is formulated as a solution to the Helmholtz equation under conditions of a time-harmonic wave and widely used to simulate the propagation of light in optical waveguides [16]. The GaN slab was surrounded by air, and the top out-coupling pattern was not introduced in this simulation. These dispersion curves exhibit important features as follows: as the thickness of GaN slab increases, higher orders of guided modes emerge in turn and the modal index of a guided mode increases gradually. The modal index changes with a variation in the thickness of the slab because it is determined by the energy distribution of a guided mode inside and outside of the slab. Also, a higher order of guided mode has a lower modal index at a fixed thickness of GaN slab. Based on these properties, one can understand that a thin GaN slab is beneficial to efficient extraction of photons because few guided modes with low modal indices are trapped in the thin slab [8]. Additionally, high orders of guided modes are extracted out efficiently because they have longer evanescent tails that enable large spatial overlap with a top out-coupling structure [5,12,17]. In contrast, low orders of guided modes are marginally perturbed by the out-coupling structure.

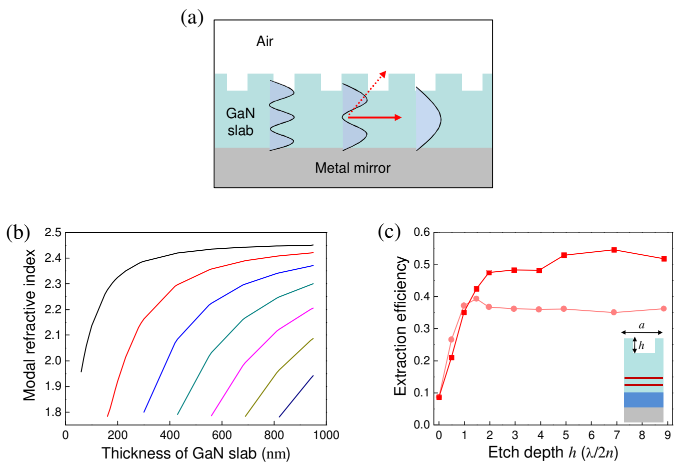

Fig. 1. (a) Schematic of several orders of guided modes that interact with the top periodic GaN pattern. (b) The calculated modal refractive index as a function of thickness of GaN slab. The uppermost plot (black curve) represents the fundamental mode. (c) Extraction efficiencies calculated as a function of etch depth of the top GaN pattern, *h*, at the lattice constant, *a*, of 240 nm (pink) and 1200 nm (red).

Although a thin GaN slab can improve light extraction significantly, a conventional vertical GaN LED has a relatively large thickness of a few microns for better electrical properties and current spreading [18]. For reference, we calculated the extraction efficiency of a conventional GaN vertical LED with a top 2D square-lattice dielectric out-coupling structure and a bottom metal mirror using three-dimensional (3D) finite-difference time-domain (FDTD) simulation (Fig. 1(c)). The thickness and refractive index of the GaN slab were set to 3 μm and 2.46, and a 60 nm-thick ITO layer was inserted between the slab and metal mirror to model an actual LED structure. Periodic boundary conditions and perfectly matched layers were used in in-plane and vertical directions, respectively. Dipole sources with a central wavelength of 450 nm and bandwidth of 25 nm were excited and the extraction efficiency was recorded at the detection plane above the GaN slab. The spatial resolution was 5 nm in the simulations. Then, the extraction efficiency was plotted as a function of the depth of the top periodic pattern, *h* (inset of Fig. 1(c)), when the pitch size, *a*, is 240 nm or 1200 nm. At a = 240 nm (pink, Fig. 1(c)), the extraction efficiency increases steadily at $h<\lambda/2n$ and plateaus with increasing depth [19,20]. On the other hand, at a = 1200 nm (red, Fig. 1(c)), the

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extraction efficiency increases constantly with increasing h and is eventually greater than the maximum extraction efficiency at a = 240 nm.

According to the phase-matching condition, a pitch size as small as ~λ/n is generally suitable to extract out low orders of guided modes occupying a large fraction of the power spectrum [5,12,17]. However, as shown in Fig. 1(c), although the pitch size of 240 nm satisfies this condition, the extraction efficiency was relatively low, which results from the narrow overlap between the fundamental mode and the top out-coupling structure. Besides this, the extraction efficiency remains nearly constant with an increase in the etch depth, because the average index in the out-coupling structure is much smaller than the modal indices of the low orders of guided modes leading to rapid attenuation of the modes in the out-coupling structure [5]. In contrast, the pitch size of 1200 nm is more effective for light extraction at h>~λ/2n. Furthermore, the simulation shows that the extraction efficiency increases with increasing h due to significant overlap between high orders of guided modes with long evanescent tails and the out-coupling pattern. Therefore, in a conventional thick GaN LED structure, it would be better to design an out-coupling pattern that can extract out high orders of guided modes. As a conclusion, to achieve high extraction efficiency from the GaN-air pattern, the pitch size and depth of the pattern are ~1 μm and > λ/2n, respectively. Nevertheless, it is still a challenging issue to investigate how to extract out low orders of guided modes, which is the current limit of extraction efficiency in LEDs.

3. Results and discussion

To extract out low orders of guided modes that are highly confined in the GaN slab, we propose a new out-coupling structure on the bottom metal mirror (Fig. 2(a)). Since silver has an abnormal complex refractive index compared to general dielectric materials, the low orders of guided modes can be easily perturbed, despite their small overlap with patterns in metal mirrors. First, in simulations, square-lattice periodic patterns consisting of ITO and perfect conductor (PC) were used for the bottom out-coupling structure. Figure 2(b) shows time-elapsed extraction efficiencies of the following three-types of vertical GaN LEDs: LEDs with no pattern (black), square-lattice periodic pattern on the top of GaN slab (red), and square-lattice periodic pattern on the PC bottom mirror (green). In the patterns introduced in the GaN-air and PC-ITO, the pitch size and pattern depth were 240 nm and 60 nm, respectively. The calculated extraction efficiencies illustrate several key features. First, for a non-patterned structure (black), the extraction efficiency was saturated at the propagation distance of ~10 μm. This implies that photons within a light cone of total internal reflection were extracted out within several round trips. Second, for both patterned structures (red and green), the extraction efficiencies increase steadily as photons bounce back and forth inside the GaN slab before all generated photons vanish by absorption loss. In case of the PC-ITO pattern, even with the small pitch size (a = 240 nm) and the shallow depth (h = 60 nm) much smaller than ~λ/n, a dramatic enhancement in extraction efficiency was achieved.

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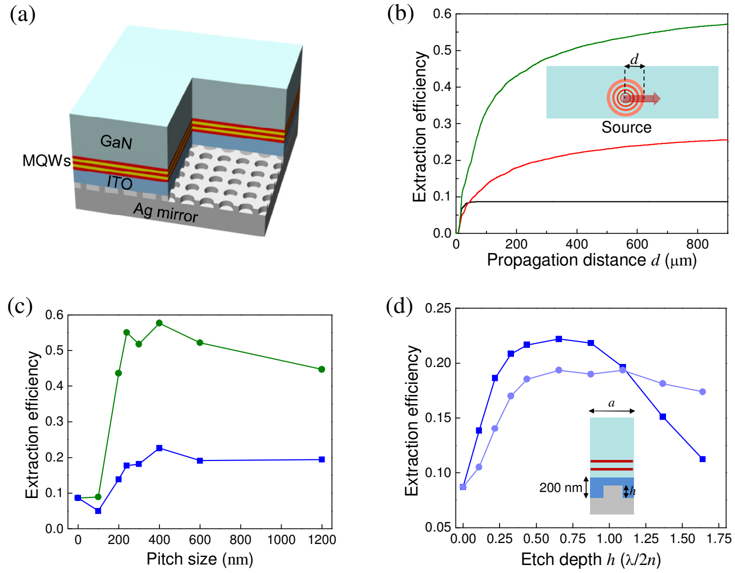

Fig. 2. (a) Schematic of a GaN vertical LED with a bottom metal-ITO patterned mirror. (b) Extraction efficiencies as a function of distance of the LEDs with no pattern (black), square-lattice periodic pattern on the top of GaN slab (red), and square-lattice periodic pattern on the PC bottom mirror (green), which were calculated as a function of light propagation distance, *d*. For all patterns, the pitch size and pattern depth were 240 nm and 60 nm, respectively. (c) Extraction efficiencies of PC-ITO patterned (green) and silver-ITO patterned (blue) GaN LEDs with varying pitch size. The pattern depth was 60 nm. (d) Extraction efficiencies of silver-ITO patterned GaN LEDs with a pitch size of 400 nm (blue) and 1200 nm (purple) calculated as a function of pattern depth.

We calculated the extraction efficiency of the metal-ITO pattern while varying the pitch size (Fig. 2(c)). As the metal component, either silver or PC was employed. Silver was modeled by the Drude model, which fits the measured dielectric function of silver in the visible spectral range. The depth of pattern was fixed at 60 nm in all structures. The simulation results show that the extraction efficiencies have maximum values at the pitch size of 200-400 nm for both metal-ITO patterns, which is much smaller than that of a dielectric out-coupling structure. This implies that the metal-dielectric patterns diffract low-orders of guided modes efficiently. The maximum enhancement in extraction efficiencies with the PC- and silver-ITO pattern were respectively 6.6 and 2.6 times higher compared to a non-patterned structure. Notably, the extraction efficiency of the PC-ITO pattern is larger than that of the GaN-air pattern (Fig. 1(c)) while the extraction efficiency was reduced significantly when the metal used was silver.

Additionally, we investigated the dependence of the extraction efficiency on the pattern depth (Fig. 2(d)). In these simulations, we examined a relatively small pitch size (a = 400 nm) and a large pitch size (a = 1200 nm) for the silver-ITO patterned structure. The total thickness of ITO was 200 nm. The result of Fig. 2(d) exhibits distinct features when compared to the result of Fig. 1(c). The maximum extraction efficiency in the silver-ITO patterned structure was observed at a much smaller depth compared to that of the GaN-air out-coupling structure. Also, the extraction efficiency begins to decrease at a depth of $>0.75\cdot(\lambda/2n)$ in case of the pitch size of 400 nm. In fact, the optimum depth of $\sim 0.75\cdot(\lambda/2n)$ providing a maximum extraction efficiency is comparable to the length of evanescent field of low-orders of guided modes.

To understand the behavior of the extraction efficiency in silver-ITO patterned structure, we calculated reflectivity as a function of the pitch size, with the relatively shallow pattern depth of 30 nm (blue, Fig. 3(a)) and the larger pattern depth of 60 nm (purple, Fig. 3(a)).

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Compared to the reflectivity of non-patterned silver mirror, the reflectivity of the silver-ITO patterned structure drops significantly from the pitch size of 100 nm, and steadily approaches the reflectivity of non-patterned silver mirror with increasing pitch size. Also, the reflectivity of the silver-ITO patterned structure increases with decreasing pattern depth over all pitch sizes. Therefore, when one designs a metal-dielectric out-coupling structure, it is necessary to consider the absorption loss that depends on the pitch size and depth in tandem with the diffraction condition. For example, low orders of guided mode are diffracted well with the pitch size of 200-400 nm, but the reflectivity of the silver-ITO patterned structure is degraded substantially at the same condition so that the resultant extraction efficiency is lower than that of the PC-ITO patterned structure (Fig. 2(c)).

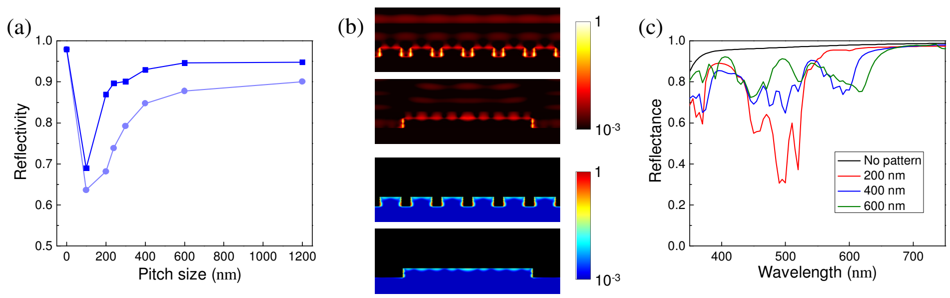

Fig. 3. (a) Reflectivity of silver-ITO patterned structures with the pattern depths of 30 nm (blue) and 60 nm (purple) which was calculated as a function of the pitch size. The structure with a pitch size of 0 nm indicates a planar silver mirror. (b) Electric field intensity (upper) and absorption intensity (bottom) in the silver-ITO structure with the pitch sizes of 200 nm and 1200 nm when a normal plane wave is incident. The pattern depth was 60 nm for both structures. (c) Reflectance of a non-patterned silver mirror (black) and silver-ITO patterned structure with the pitch sizes of 200 nm (red), 400 nm (blue) and 600 nm (green). For the silver-ITO patterned structure, the depth of pattern was 60 nm.

To investigate the origin of absorption loss in a silver-ITO patterned structure, an electric-field intensity distribution (top, Fig. 3(b)) and absorption intensity distribution (bottom, Fig. 3(b)) were calculated. In these simulations, a normal plane wave with a monochromatic wavelength of 450 nm is used and the absorption is calculated by integrating $J \cdot E$ over one optical cycle, where J and E are the polarization current density and electric field, respectively. The snapshots reveal that a noticeable portion of incident photons are coupled to plasmonic modes which are highly concentrated at the interface between silver and surrounding dielectric material. In particular, stronger absorption takes places at the structure with a smaller pitch size (a = 200 nm). Thus, one can conclude that the absorption in the metal-dielectric pattern stems from plasmonic absorption loss that depends on the pitch size of metal-dielectric pattern as well as bulk plasmonic frequency [21–23]. Figure 3(c) shows reflectance spectra of a silver-ITO patterned structure with pitch sizes of 200 nm (red), 400 nm (blue) and 600 nm (green). Although all the spectra exhibit complex wavelength- and pitch-size-dependent resonances that are given by the plasmon excitation condition, the overall reflectance approaches the value of non-patterned structure (black, Fig. 3(c)) as the wavelength is increasingly far from the plasmonic frequency of bulk silver.

Lastly, we propose a double-sided out-coupling structure in the GaN vertical LED (Fig. 4(a)). This structure consists of an upper GaN-air pattern and a bottom metal-ITO pattern, where metal is either silver or PC. In simulations, the pitch size and depth of the metal-ITO pattern were varied, whereas the pitch size and depth of the GaN-air pattern were fixed to 1200 and 675 nm, respectively. The calculated extraction efficiency in the structure with the double-sided patterns reveals distinguishable features from the structure with the single upper GaN-air pattern (Fig. 4(b)). For example, in the structure with the PC-ITO and GaN-air out-coupling patterns (green, Fig. 4(b)), the extraction efficiency was enhanced by ~40% as compared to the structure with the reference GaN-air pattern with a = 1200 nm and h = 675 nm. However, the extraction efficiency in the structure with the silver-ITO and GaN-air

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patterns (blue, Fig. 4(b)) increased with increasing the pitch size, but the maximum efficiency was still lower than that in the structure with the reference GaN-air pattern. Hence, one can understand that the extraction efficiency of the silver-ITO and GaN-air patterns was primarily determined by the absorption loss from the silver-dielectric out-coupling structure, rather than diffraction of low orders of guided modes. Hence, the double-sided out-coupling structure will show an enhancement in extraction efficiency if the plasmonic absorption loss at the metal surfaces is minimized. For example, for red or infra-red emitting LEDs, the double-sided out-coupling structure with aluminum instead of silver would be beneficial since aluminum has lower bulk plasmonic frequency than silver [24]. Although a metal-dielectric out-coupling structure together with a conventional dielectric pattern may offer a new route to enhance light extraction at discrete or a broad range of emission wavelengths, further study will be necessary to achieve an overall enhancement in extraction efficiency while minimizing plasmonic absorption loss at the metal surface.

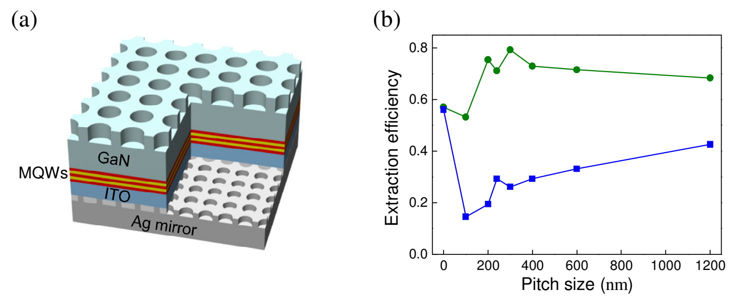

Fig. 4. (a) Schematic of a GaN vertical LED with double-sided out-coupling patterns consisting of a top GaN-air and a bottom metal-ITO patterns. (b) Extraction efficiency of double-sided patterns as a function of the pitch size of metal-ITO pattern, where metal is either PC (green) or silver (blue). The origin in this plot implies the structure with single GaN-air pattern. The pitch size of GaN-air pattern was 1200 nm.

4. Conclusion

A metal-dielectric pattern in GaN vertical LEDs is useful to enhance the extraction efficiency by converting low orders of guided modes into leaky continuum modes. The optimum pitch size of a metal-ITO pattern ranges from 200 to 400 nm, which is distinguishable from a GaN-air pattern with an optimum pitch size of ~1 μm. Also, the extraction efficiency further increases with depths of <100 nm of a metal-ITO pattern, which is similar to the effective range of the evanescent field of extracted guided modes. In the structure with an optimized PC-ITO pattern, the extraction efficiency was 6.6-fold enhanced compared to a non-patterned structure. On the other hand, in the structure with a silver-ITO pattern, the enhancement factor of efficiency was reduced to 2.6 due to plasmonic absorption loss. A double-sided out-coupling structure with top GaN-air and bottom metal-dielectric patterns was proposed as an ultimate light extractor. Compared to the structure with single GaN-air pattern, the double-sided pattern with a PC-ITO pattern yielded a 40% enhancement in extraction efficiency, whereas the efficiency of the double-sided pattern with a silver-ITO pattern was degraded due to the plasmonic absorption loss. The understanding of a metal-dielectric pattern will be useful for the demonstration of efficient in- and out-couplers, scattering elements and absorbers-based subwavelength metallic structures that can be embedded in various optoelectronic applications.

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