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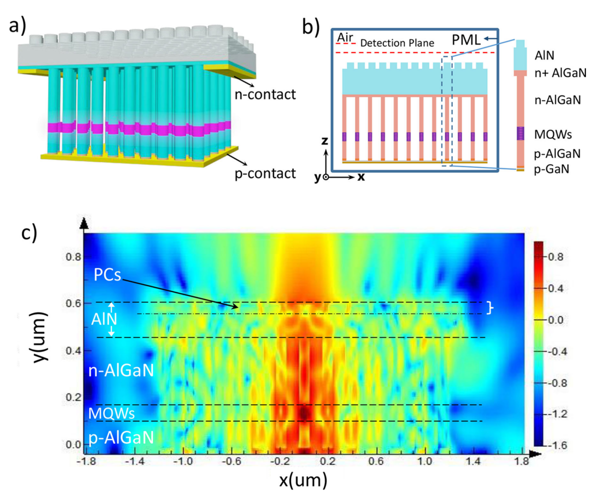

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Enhancing Light Extraction Efficiency of Vertical Emission of AlGaN Nanowire Light Emitting Diodes With Photonic Crystal

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Abstract: AlGaN alloys have been widely used to make ultraviolet light-emitting diodes (UV-LEDs) because its energy bandgap covers 200–360 nm wavelength range. However, AlGaN shows strong transverse magnetic polarization in deep UV range, which severely prevents light extraction from top surface of UV-LEDs. In this paper, we propose a novel flip-chip AlGaN nanowire LED with top photonic crystals, for the purpose of improving light extraction efficiency (LEE) from top surface. Using three-dimensional finite-difference time domain simulation, we first investigate the LEE in vertical direction of nanowire LEDs. By carefully optimizing the size and density of nanowires, we demonstrate that nanowire structures can be designed to inhibit the emission of guided mode and promote light extraction from top surface. Based on the optimized nanowire structure, we also study the effect of top photonic crystals on the LEE of vertical emission. A high LEE up to 79.4% can be achieved by optimizing the height, spacing, and radius of top photonic crystals. Analyzing the lateral electric field distribution of AlGaN nanowire LEDs with and without top photonic crystals, we find that top photonic crystals can effectively improve the LEE of vertical emission by coupling the light trapped in epitaxial layers out of LEDs.

Index Terms: Light emitting diodes, ultraviolet, AlGaN nanowire, light extraction, vertical emission, photonic crystal.

1. Introduction

AlGaN-based ultraviolet light-emitting diodes (UV LEDs) have attracted significant attention recently as new UV light sources for various applications such as water purification [1], biological sensing [2], and disinfection [3]. However, high performance UV-LEDs are still scarce. The external quantum efficiency of conventional AlGaN quantum wells (QWs) UV-LEDs is severely limited due to very low light extraction efficiency (LEE), about 10% [4]–[6]. There are several issues leading to the poor LEE. The first is the severe photons confinement due to very high total internal reflection (TIR) [7]. For conventional planar LEDs, only very small amounts of light within the escape cone can escape to the outside of the device [8]. The rest of light will be trapped inside the epitaxial layers due to TIR. The second issue is the high absorption of p-GaN and metal contact layer [9], [10]. In

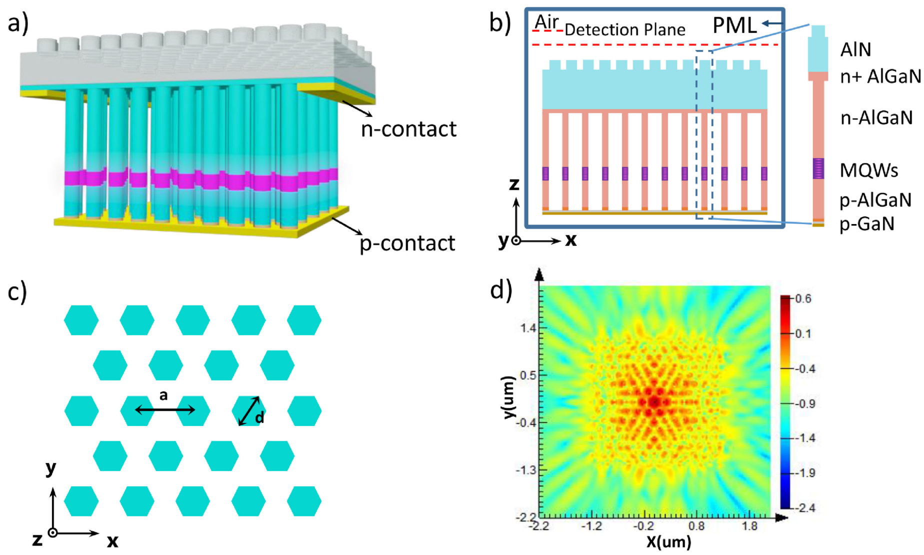

Fig. 1. (a) 3D Schematic illustration and (b) 2D cross-sectional schematic illustration of the x-z plane of the proposed novel LED structure in this work. (c) 2D cross-sectional schematic illustration of the x-y plane of the nanowire array and (d) the simulated optical mode profile for nanowire LEDs with the spacing(a) ∼190 nm and radius ∼42 nm.

addition, AlGaN-based LEDs with high Al composition show unique polarization performance. In the wurtzite form, GaN has a positive crystal-field splitting energy($E_{CEF} = +38$ meV), therefore light emission is transverse electric(TE) polarized. However, AlN has a negative crystal-field splitting energy($E_{CEF} = -219$ meV), which makes the order of the valence bands in AlN different from that in GaN. As a result, light emission is transverse magnetic (TM) polarized in AlN [11], [12]. Light emitted from AlGaN active region has two optical polarization modes: TE mode and TM mode [13]. The polarization of the TE and TM mode corresponds to the electric field direction perpendicular and parallel, respectively, to the c axis, which is also defined as the nanowire growth direction in this study [14]. With the increase of Al component, TM polarization becomes dominant because the material properties of AlGaN are getting closer to AlN. As a consequence, most of the emitted light can only propagate horizontally, which prevents the light extraction from top surface [15].

Recently, quantitative analyses on various LED structures such as patterned sapphire substrate [16], [17], surface roughening [18], [19] and surface plasmon [20], [21] have been proposed and developed to improve LEE of planar UV LEDs. Despite these numerous efforts, achieving high efficiency AlGaN-based planar UV LEDs still remains challenging. On the other hand, nanowire structures have been reported to realize high efficiency LED with lateral emission because of horizontal propagation characteristic of TM polarization [22]. However, the total area of lateral emission is very limited due to the small lateral area of UV LEDs. Therefore, it is more desirable to extract light from the top surface. Nevertheless, there are few reports achieving high LEE on top surface for TM polarized AlGaN-based LEDs.

In this study, we propose a novel LED structure for the purpose of improving LEE of vertical emission. This novel LED, as shown in Fig. 1(a), is a flip-chip nanowire structure with top photonic crystals. Photonic crystals have superior optical mode control and can efficiently couple guided modes out of the LEDs [23]. By using the 3D finite difference time-domain (FDTD) simulation, we investigate the LEE from top surface of UV nanowire LEDs and the effect of top photonic crystals layer on LEE. Compared to the conventional LEDs, this LED has several advantages. Firstly, since the top surface has no metal contact, the absorption of light by metal contact layer can be effectively avoided [24]. More importantly, our simulation shows that this structure can promote vertical light emission from top surface with the addition of top AlN photonic crystal, and the LEE can be significantly enhanced by optimizing the spacing and radius of nanowires and the spacing, radius and height of AlN photonic crystals.

This novel LED structure can be fabricated with the following process. Firstly, a thick planar AlN layer is epitaxially grown on sapphire substrate, followed by a n+AlGaN thin layer. Then nanowire LED arrays are grown on top of n+AlGaN thin layer by molecular beam epitaxy. The top p-metal contact is deposited directly on top of the nanowire array using a tilt-angle deposition [25], [26]. After p- and n-contacts are deposited, the above entire structure is flip-chip mounted on Au-coated SiC submounts, and the original sapphire substrate is removed using pulsed UV laser irradiation [27]. Finally, we make a layer of AlN pillar photonic crystals on the top portion of the AlN layer by ICP etching [28].

2. Simulation Details

Fig. 1(b) shows the structure parameters we used in this work. Each nanowire consists of 10 nm p-GaN, 100 nm p-$Al_{0.5}Ga_{0.5}N$, 60 nm undoped $Al_{0.6}Ga_{0.4}N/Al_{0.4}Ga_{0.6}N$ active region and 300 nm n-$Al_{0.5}Ga_{0.5}N$. The cross section of nanowire array is a hexagonal geometry, as shown in Fig. 1(c).The spacing$\sim$ a is defined as the center to center distance between two adjacent nanowires. On top of nanowire array, the heavily doped n+AlGaN layer is 10 nm thick. Doping concentration and sheet resistance of n+AlGaN layer are 2×10^{19} cm^{-3} and 160$\Omega/\square$, respectively [29]. Because the AlGaN layer is very thin($<$500 nm), the relaxation ratio of AlN and AlGaN is assumed to be 3% [30]. The total thickness of AlN layer is set to 140 nm. Some photonic crystals are etched on the upper surface of the AlN layer. The refractive indexes and absorption coefficients for GaN, AlGaN and AlN used in this work are taken from refs [15], [31]. As for the bottom metal electrode which is also a reflective layer, we use metal boundary conditions as a perfectly reflective layer [32]. Considering the trade-off between computing power and simulation accuracy, the simulated LED domain is 2.5 um $\times$ 2.5 um. In order to avoid the undesired reflection of boundaries, the perfect matched layers (PMLs) are used as absorbing boundaries around the simulated structure [33]. We employ 12 PMLs to absorb outgoing light. There is a 1 um distance between PMLs and the simulated structure so as to avoid the adverse impact of PMLs on simulation results. Lumerical adaptive meshing is used in our simulation. The size of spatial grids will be automatically adjusted according to the structure. In other words, the mesh can be assigned relatively large when the material is uniform and constant. On the contrary, when the structure size changes greatly, the mesh will automatically decrease to ensure the simulation accuracy. The minimum mesh step is 0.25 nm, which is small enough for our simulated structure.

In the FDTD simulation, a single dipole source is positioned in the middle of active region, which is a commonly used approach in LED simulation [22], [34], [35]. Although a single dipole source is placed at the central nanowire in the simulation region, the electric field can effectively spread across the entire LED structure due to the periodicity of nanowires array, as shown in Fig. 1(d). In addition, using multiple dipole sources to perform simulation is not an appropriate method. Because multiple dipole sources will result in non-physical interference pattern, which is undesirable for analysis of optical properties of LEDs [36]. The AlGaN active region can emit light in both TE and TM mode. However, TM mode is dominant at 280 nm or shorter wavelengths [22], [37]. In this work, the wavelength used for simulation is 280 nm and we assume that the light emission of active region is 100% TM polarized. The spectrum of TM dipole source has a Gaussian shape. The LEE of top surface is defined as the ratio of the emitted power going upward within a rectangular region above the AlN layer to the total power of the active region [38], [39]. In this work, we use a power monitor, which is a sufficiently large rectangular plane, to collect the light escaping from the top surface of the LED device. And a power monitor analysis group surrounding the dipole source is used in our simulation to measure the total power generated in active region.

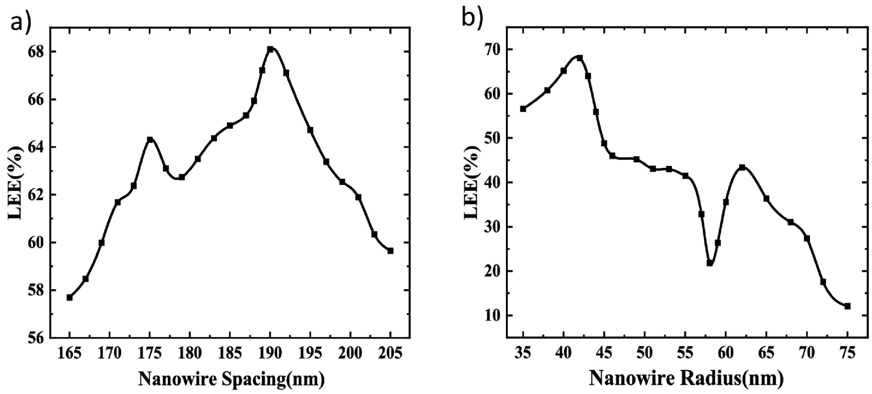

Fig. 2. (a) LEE versus nanowire spacing with nanowire radius of 42 nm. (b) LEE versus nanowire radius with nanowire spacing of 190 nm.

3. Results

We firstly investigate the dependence of LEE on the radius and the spacing of nanowires before the AlN photonic crystal pillars are etched into the top portion of the AlN layer. The spacing is defined as the distance from center to center of adjacent nanowires. Particle swarm optimization (PSO) algorithm is used for parameter optimization [40]. The PSO, as one of advanced algorithms, is widely used in various optimization problems such as filter [41] and array antenna designs [42]. We set up ten iterations, and each has ten particles. In other words, a total number of 100 times simulations are performed. A maximum LEE of 68% is achieved, which is calculated for nanowire spacing of 190 nm and radius of 42 nm. To better understand the relationship between the LEE and nanowire spacing, we set the radius of the nanowire at 42 nm, and then sweep the nanowire spacing from 165 nm to 205 nm. The relationship between LEE and nanowire spacing is shown in Fig. 2(a), which varies from 57.6% to 68%. This result shows that the photonic confinement effect plays a major role with relatively small nanowire spacing, which deteriorates the LEE. Increasing nanowire spacing, the LEE gradually improves and eventually reaches the maximum due to the coupling to vertical emission [43]. As for the pit at 178 nm in Fig. 2(a), this is due to the formation of closed-loop optical path. Under proper configuration, adjacent nanowires can form a closed loop. Light will be confined to the closed loop path and scattered multiple times by AlGaN nanowires, which is not conducive to vertical emitting [44]. Furthermore, the propagation of light in the closed-loop path also increases the optical absorption by materials. Increasing nanowire spacing further($>$190 nm), it becomes easy for TM mode light propagating horizontally through the nanowire array and vertical couple mode becomes weak, leading to a decrease of LEE in vertical direction.

We keep the optimal nanowire spacing at 190 nm and sweep the nanowires radius from 35 nm to 75 nm, for the purpose of studying the relation between LEE and nanowires radius. Fig. 2(b) plots the variation of LEE with increasing the radius of nanowires. For relatively small nanowire radius, the LEE is generally high, and reaches the maximum when the nanowire radius is 42 nm. Although light is more likely to escape from the small radius nanowire, Nanowires with very small radius ($<$35 nm) are not desirable because they cannot support coupled modes. In addition, small radius nanowire will reduce the volume of active region, resulting in low output power. The LEE shows a decreasing trend with further increasing nanowire radius($>$42 nm). Because light has to travel a longer distance through the large radius nanowire, and consequently, light will be absorbed more heavily by nanowire materials. The sudden decrease of LEE occurs at 57.5 nm. This is because the energy band redshifts with increasing nanowire radius, and the operating wavelength is close to the M point [43]. As a result, the coupling efficiency in vertical direction becomes less efficient.

We also study the LEE of normal chip nanowire LED, in order to prove that the flip-chip structure can improve light extraction. The 2D schematic illustration of the normal chip is shown in Fig. 3(a). The height of each layer in the nanowire of normal chip is the same as the flip-chip structure

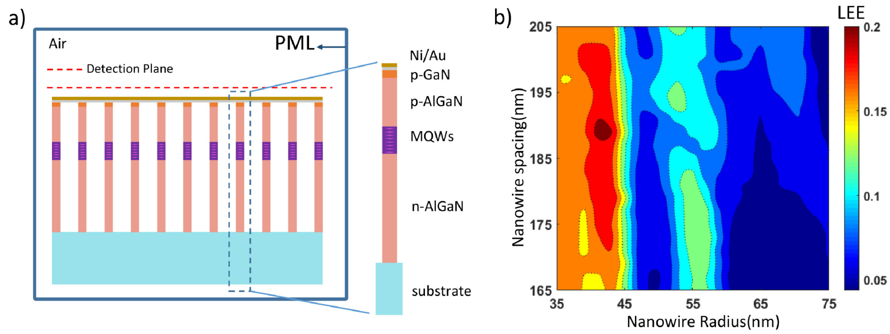

Fig. 3. (a) 2D cross-sectional schematic illustration of the normal chip LED. (b) Contour map of the LEE of normal chip nanowire LED vs. nanowire spacing and radius.

proposed in this paper. On top of p-GaN layer, we use Ni/Au(10 nm/10 nm) to make metal contact. Light is extracted from the upper surface(p-side). Fig. 3(b) is the contour map of the LEE of normal chip vs. the nanowire spacing and radius. It is seen that, LEE is generally low, and the highest value is only 20%. The main reason is the severe light absorption from p-GaN and top metal electrode. Through the comparison with the normal chip, it can be proved that our flip-chip nanowire structure is helpful for improving the LEE.

To gain more insight into how nanowire structure improves the LEE, we contrast the lateral electric field distribution of nanowire LED in TM mode with a conventional planar LED. The simulated result is plotted in Fig. 4(a) and (b). The thickness of each layer of the planar LED is equal to that of the nanowire LED. The spacing and radius of nanowires are kept at optimal values of 190 nm and 42 nm, respectively. Shown in Fig. 4(a), the electric field is mainly distributed within the epitaxial layers for planar LED with a trend of horizontal propagation. This is due to the strong TIR effect. In this case, light generated from active region will become guided mode and is hard to escape from the planar LED. For the nanowire LED in Fig. 4(b), on the contrary, electric field is distributed vertically, and the horizontal propagation is weaker than the planar LED. This is because the array nanowire structure diffracts the light generated from active region, making more light into radiation mode. It's worth mentioning that the electric field intensity of nanowire LED is relatively high above the AlN layer, in contrast with the situation in planar LED. This indicates that nanowire structures can be designed to inhibit the guided modes and redirect light into radiated modes [45]. As a result, the light generated from active region can effectively escape from the top surface of nanowire LED.

Based on the optimized nanowire LED structure shown above, we add photonic crystal pillars into the top portion of the planar AlN layer, investigating the effect of photonic crystals on LEE. Firstly, we use PSO to optimize the parameters including the height, radius and spacing of photonic crystals. Because we focus on the effect of surface photonic crystals, we choose a sweep range of 0–60 nm for the height of photonic crystals. Photonic crystals radius is swept from 45 nm to 85 nm. And the spacing range of photonic crystalss is from 170 nm to 220 nm. During the optimization of photonic crystals parameters, the spacing and radius of nanowire LED are kept at 190 nm and 42 nm, respectively. Through detailed simulations, a maximum LEE of 79.4% can be achieved, with a spacing of 182 nm, a radius of 75 nm and a height of 32 nm.

We keep the spacing of photonic crystals at 182 nm and the radius of photonic crystals at 75 nm, then study LEE as a function of the photonic crystal height. Fig. 5(a) shows the relation between LEE and the height of photonic crystals. Increasing the height of photonic crystals from 0 nm (no photonic crystals) to 20 nm, LEE has a big boost. This is due to the coupling of photonic crystals [46]. Further increasing the photonic crystal height, LEE shows a gently increasing trend and then reaches the maximum at the height of 32 nm. Afterward, when the height increases further from 32 nm to 60 nm, LEE decreases from 79.4% to 69.3%. This is probably due to the fact that more and more light is confined between the pillars of AlN photonic crystals.

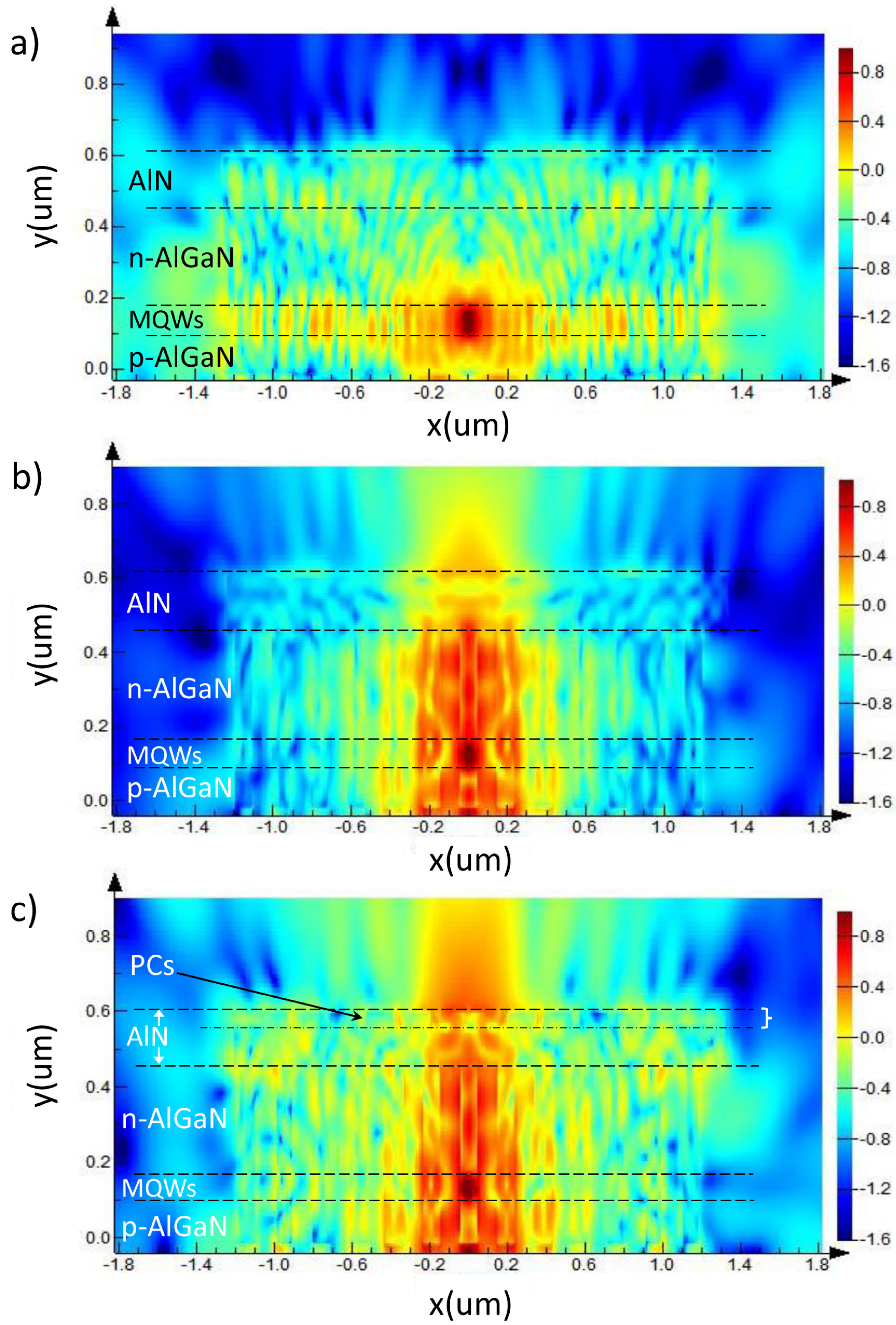

Fig. 4. Lateral electric field distribution for TM mode of (a) planar LED, (b) nanowires LED without photonic crystals and (c) nanowires LED with photonic crystals. The radius and spacing of nanowires are 42 nm and 190 nm respectively for three devices. The height, radius and spacing of pillar photonic crystals are 32 nm, 75 nm and 182 nm, respectively.

Fig. 5(b) shows the relation between LEE and the radius of photonic crystals when the height of the photonic crystals is 32 nm and the spacing is 182 nm. Changing the photonic crystals radius from 45 nm to 75 nm, LEE increases and reaches the maximum at 75 nm. However, LEE decreases rapidly as the radius further increases. The relationship between LEE and photonic crystals spacing is shown in Fig. 5(c). The height and radius of photonic crystals are kept at 32 nm and 75 nm,

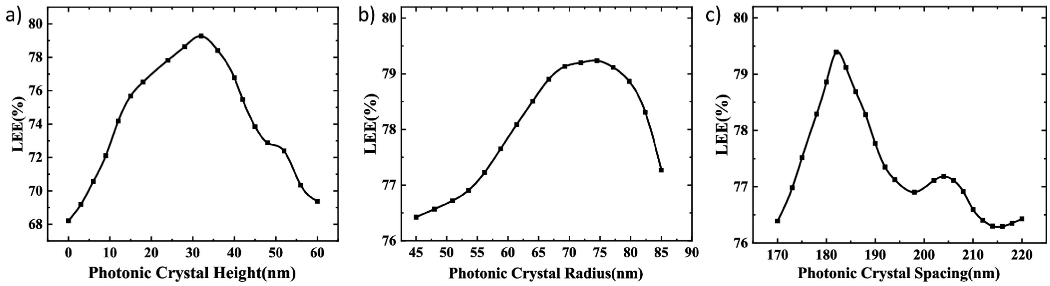

Fig. 5. (a) LEE vs. the height of AlN photonic crystals with optimized nanowire parameters. The photonic crystals radius and spacing is kept at 75 nm and 182 nm, respectively. (b) LEE vs. the radius of photonic crystals with optimized nanowire parameters. The photonic crystals height and spacing is kept at 32 nm and 182 nm, respectively. (c) LEE vs. the spacing of photonic crystals with optimized nanowire parameters. The photonic crystals height and radius is kept at 32 nm and 75 nm, respectively.

respectively. The photonic crystal spacing changes from 170 nm to 220 nm. Corresponding LEE changes from 76% to 79.4%. As the spacing of photonic crystals gradually increases from 170 nm to 183 nm, LEE shows a rising tendency due to the formation of coupled modes [47]. However, as the photonic crystal spacing increases further, the coupled modes are broken, resulting a decrease of LEE.

In order to gain a more comprehensive understanding of how top photonic crystals(PCs) improve the LEE, we contrast the lateral electric field distribution with and without photonic crystals, as shown in Fig. 4(c) and 4(b), respectively. Here, the radius of nanowires is 42 nm and the spacing of nanowires is 190 nm in both structures. In addition, for the LED with photonic crystals, shown in Fig. 4(c), we keep the height, radius and spacing of AlN pillar photonic crystals at 32 nm, 75 nm and 182 nm, respectively. It can be seen from Fig. 4(b), the lateral electric field distribution of LED without top photonic crystals, that the electric field intensity above the AlN layer is weaker than the LED with photonic crystals in Fig. 4(c). The refractive indices of AlN photonic crystals and the surrounding air are very different, which can produce strong Bragg diffractions on the light trapped in AlN layer. Contrasting Fig. 4(b) with Fig. 4(c), we can see clearly that the electric field intensity above AlN layer can be enhanced by adding top photonic crystals.

4. Conclusions

In summary, we report a novel flip-chip nanowire LED with top photonic crystals and have investigated its vertical emission properties using 3D FDTD simulation. Because this LED structure does not have the metal electrode on the top surface, the absorption of light by top electrode can be avoided. In addition, we effectively inhibit the guide mode and redirect into the radiation mode by using the nanowire structure, which allows more light trapped in epitaxial layers to escape from the device. More importantly, by adding a top AlN photonic crystals layer, we enhance the light emission from the top surface, leading to LEE's further ascent. We achieve a 79% LEE of vertical emission by optimizing the size, density of the nanowire LEDs and the size, spacing and height of top photonic crystals. This study provides a valuable inspiration for designing high performance optoelectronic devices operating in deep UV wavelength region.

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