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Antireflective sub-wavelength structures for improvement of the extraction efficiency and color rendering index of monolithic white light-emitting diode

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Abstract: We have theoretically investigated the influence of antireflective sub-wavelength structures on a monolithic white light-emitting diode (LED). The simulation is based on the rigorous coupled wave analysis (RCWA) algorithm, and both cylinder and moth-eye structures have been studied in the work. Our simulation results show that a moth-eye structure enhances the light extraction efficiency over the entire visible light range with an extraction efficiency enhancement of up to 26 %. Also for the first time to our best knowledge, the influence of sub-wavelength structures on both the color rendering index (CRI) and the correlated color temperature (CCT) of the monolithic white LED have been demonstrated. The CRI of the monolithic white LED could be improved from 92.68 to around 94 by applying a cylinder structure, and the CCT could be modified in a very large range with appropriate design of the cylinder structure.

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1. Introduction

To date, white light-emitting diodes (LEDs) are the most promising technologies for illumination market to replace conventional incandescent lamps, as energy-saving and environment-friendly light sources. It is well known that the efficiency of LEDs is determined by the product of the internal quantum efficiency and light extraction efficiency. Extremely high internal quantum efficiency close to 100 % could be achieved, however, the light extraction efficiency is usually low due to the internal reflection loss arising from large refractive index difference between semiconductor materials and air interfaces. As a result, enhancement of the light extraction efficiency becomes especially important in LEDs applications.

Various approaches have been proposed to enhance the light extraction efficiency of LEDs during the last decades. Traditionally, a single-layer quarter-wavelength thin-film antireflection coating can be applied to enhance the lighting for a specific wavelength at very low level. Broadband application can be achieved by applying a stack of antireflection coatings with appropriate design [1, 2], however, it is usually limited by the availability of materials with appropriate refractive indices and thermal expansion coefficients [3]. Meanwhile, methods relying on random light redirecting such as surface roughening have been employed [4, 5], and increasing research effort have been intensively devoted to the antireflection coating based on sub-wavelength structures such as photonic crystal [6–10], nanorod [11–14], and moth-eye structure [3, 15, 16]. Although antireflective sub-wavelength structures have been proved as an ideal method to enhance the light transmittance over a broad spectral bandwidth among all these

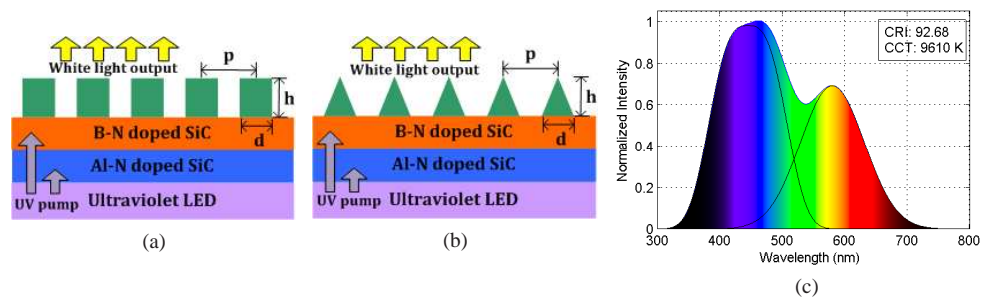


Fig. 1: Schematic cross-section of modeled monolithic white LED (a) with cylinder structure, (b) with moth-eye structure, and (c) simulated spectrum with two peaks for Al-N emission and B-N emission respectively. The Al-N emission is simulated as a 1.5 order Gaussian distribution and B-N emission is simulated as a standard Gaussian distribution.

methods, how these structures affect the color rendering index and correlated color temperature of white LEDs has never been systematically studied.

A new monolithic white LED structure consisting of two 6H-SiC layers which are co-doped with Al and N in the first layer and B and N in the second layer has been proposed by Kamiyama [17–19]. By applying optical pumping at ultraviolet (UV) range, the combined broad donor to acceptor pair (DAP) band luminescence from these two SiC layers can cover most visible wavelengths, thus white light can be produced with a high color rendering index. Despite the fact of SiC being as indirect bandgap material, high internal quantum efficiency has been obtained from this DAP luminescence which is probably due to the large medium volume for optical pumping [17]. Moreover, SiC is a well-established substrate material for nitride growth and has excellent thermal conductivity. In the present work, we theoretically investigated how antireflective sub-wavelength structures affect the white light spectrum generated by Kamiyama LED in respects of the light extraction efficiency, color rendering index, and correlated color temperature. Both cylinder and moth-eye structures have been studied in the simulation based on the rigorous coupled wave analysis algorithm [20].

2. Simulation of different structures

The simulation is based on the two dimensional RCWA (2D-RCWA) algorithm, and both moth-eye and cylinder structures are arranged in the hexagonal grid. In the simulation of moth-eye structure, the structure array is approximated by a stack of 100 horizontal layers with increasing radii from air to the substrate. The reflectance of the whole system is obtained by solving the Maxwell equation in each layer and matching the electromagnetic boundary conditions between neighboring layers from the RCWA calculations. Meanwhile, the cylinder structure array has been considered as a single layer with certain refractive index and radius in the simulation. In both structures, the grating period is defined as p and is the distance between the centers of the neighboring structures, d is the width of the structure, and h is the height of the structure (illustrated in Fig. 1a and 1b). Since structure width has very weak influence on the light transmittance [3, 15, 21], fixed values of $d=120$ nm and $p=1.4d$ have been applied as optimized profile in all the following simulations. The working wavelengths were set to the whole visible light range from 360 nm to 800 nm. Based on the validity confirmation, normal light incidence to the surface was applied for the simplification. The structure height varied from 0 to 800 nm in steps of 5 nm.

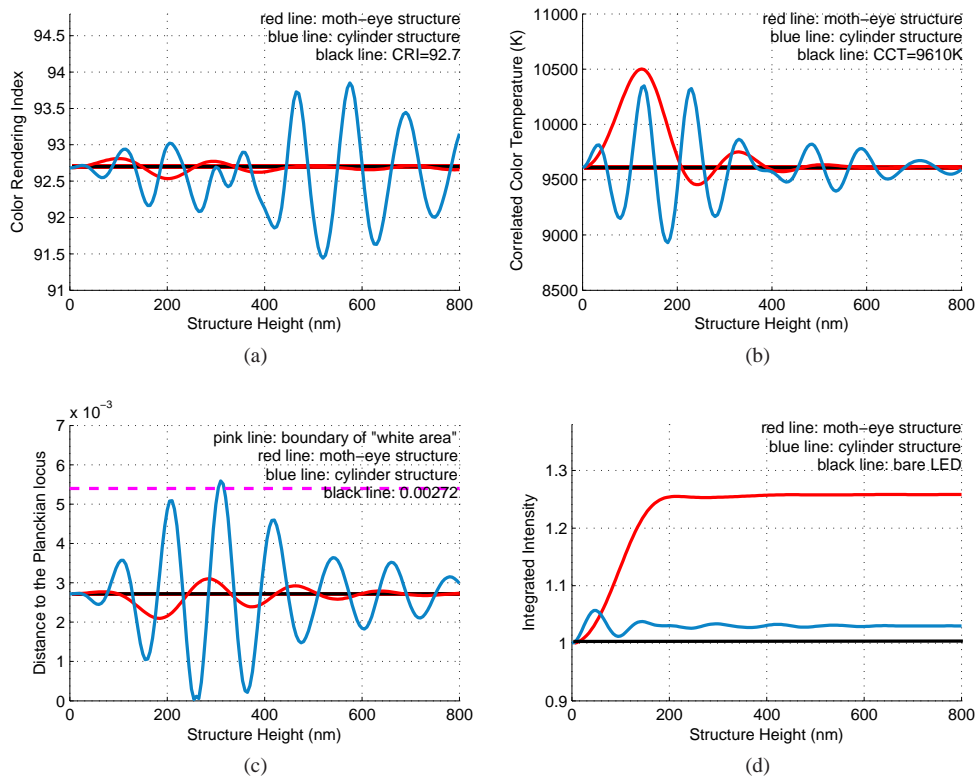


Fig. 2: (a) CRI, (b) CCT, (c) distance to the Planckian locus, and (d) integrated intensity of cylinder (blue line) and moth-eye structures (red line) as functions of the structure height.

According to the preliminary experimental results, the B-N doped SiC layer could produce a broad DAP luminescence peaked at 580 nm with a full width at half maximum (FWHM) of 120 nm. In addition, the Al-N doped SiC layer could also produce a broad DAP luminescence with similar FWHM but the peak wavelength varies between 420 and 460 nm depending on the doping level. We first simulated these two luminescence peaks with best fit to the experimental results (1.5 and 1 order Gaussian profile for Al-N and B-N DAP luminescence, respectively). Its combination has a maximal CRI of 92.68 with a CCT of 9610 K (see Fig. 1c), and its distance to the Planckian locus in the chromaticity diagram is only 2.72×10^{-3} .

The final transmitted spectrum is achieved by the product of the simulated spectrum and the transmittance curves. By changing the structure type and varying the structure height, different transmittance curves could be obtained, thus the variation of CRI, CCT, distance to the Planckian locus, and the integrated intensity over the entire visible light range of the final transmitted spectra could be calculated. All these results have been shown in Fig. 2. From Fig. 2a, it is found that cylinder structure could affect the CRI in the range of ± 1.2 while moth-eye structure only affect the CRI in the range of ± 0.2 . The highest CRI value which closes to 94 was achieved in a cylinder structure. Similar phenomenon has also been observed in Fig. 2b. With the same structure height, cylinder structure could affect the CCT value much more dramatically than the moth-eye structure. In general, any point in the chromaticity diagram whose distance to the Planckian locus is within 5.4×10^{-3} is defined as "white color". According to this definition,

Table 1: Comparison of three examples: (a) none structure, (b) highest CRI, and (c) highest intensity in terms of CRI, CCT, DC, chromatic coordinates, intensity, structure, and height

	CRI	CCT (K)	DC	(x,y)	Intensity	Structure	Height (nm)
a	92.68	9609	0.0027	(0.2845, 0.2877)	100 %	None	0
b	93.84	9731	0.0027	(0.2837, 0.2869)	102.9 %	Cylinder	575
c	92.60	9593	0.0029	(0.2847, 0.2876)	125.8 %	Moth-eye	450

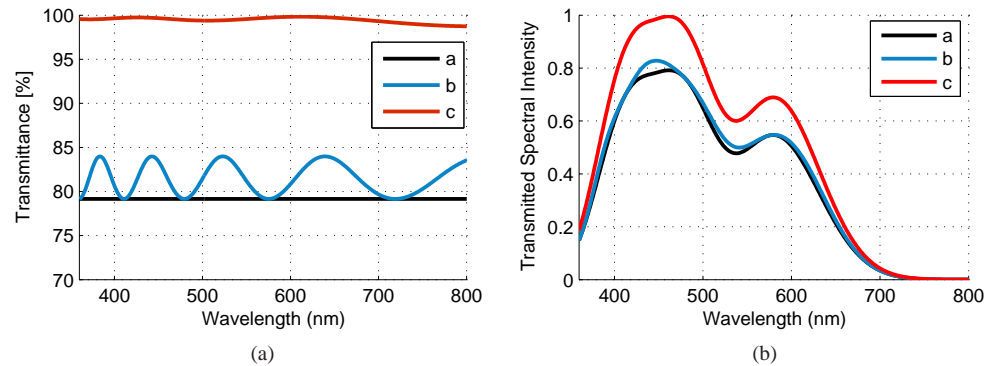


Fig. 3: (a) Transmittance curves, and (b) transmitted spectra of the three examples a, b, and c listed in table. 1

almost all the transmitted spectra of both structure types are located in the “white area” in the chromaticity diagram only except a few examples for the cylinder structure (see Fig. 2c). The integrated intensities of the transmitted spectra over the entire visible range for both structure types have been calculated and results are shown in Fig. 2d. All the calculated results are normalized to the one without any structure applied. It is obviously shown that moth-eye structure could improve the light extraction efficiency as high as 25.8 %, which is much larger than the typical value of cylinder structure (2-3 %).

3. Optimized design for extraction efficiency and color rendering index

Among the simulation results, three examples have been selected and summarized in table 1. The CRI, CCT, distance to the Planckian locus (DC), (x, y) coordinate in the CIE 1931 chromaticity diagram, integrated intensity over the entire visible range, structure type, and structure height of these three examples have been compared. There is no structure applied for example a. Example b has the highest CRI of 93.84, and the extraction efficiency is 2.9 % higher than that of example a, which was achieved in a cylinder structure with height of 575 nm. The highest extraction efficiency improvement of 25.8 % was achieved in example c which was a moth-eye structure with height of 450 nm. Its CRI value is almost the same as example a.

Transmittance curves and transmitted spectra of these three examples have been plotted in Fig. 3. Fig. 3a shows that the overall transmittance of the moth-eye structure is much larger than that of cylinder structure, which is in good accordance with the results from Fig. 2d. Example b has a local maximum at around 440 nm in its transmittance curve and it enhances the transmittance of this area relatively larger than others (see Fig. 3b). We attribute this to one of the crucial reasons which lead example b to have the highest CRI.

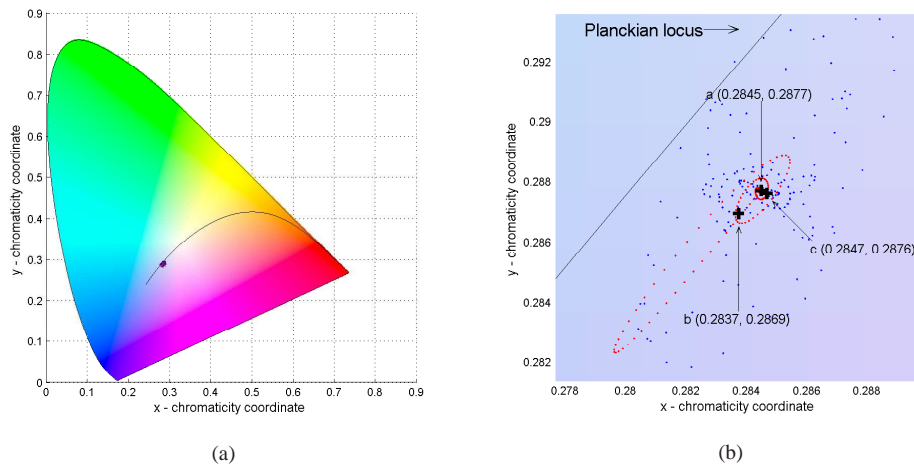


Fig. 4: (a) Locations of all the transmitted spectra in CIE 1931 (x, y) chromaticity diagram, and (b) zoom-in for examples a, b, and c, where blue and red dots stand for the cylinder and moth-eye structures with varied structure height, respectively.

Fig. 4a shows the locations of all the transmitted spectra in CIE 1931 (x, y) chromaticity diagram. Fig. 4b is the zoom-in area where the positions of example a, b, and c are highlighted. Blue and red dots stand for the cylinder and moth-eye structures with varied structure height respectively. Blue dots have relatively wider distribution than red dots, so the distance of to the Planckian locus is varied in a larger level, which agrees with the results observed in Fig. 2c. In addition, cylinder structure shows the ability to obtain much lower CCT, and CCT value as low as 8930 K could be obtained. Nevertheless, the positions of the example a, b, and c are very close to each other, and all of the three examples have almost the same distance to the Planckian locus.

4. Conclusion

From our simulation, moth-eye structure could lead to very large light extraction efficiency with improvement as high as 25.8 %, and the influence of structure dimensions on CRI and CCT is insignificant especially when the structure height is larger than 400 nm. Meanwhile, the highest CRI of around 94 could be achieved in a cylinder structure with structure height of 575 nm, the light extraction efficiency has only been enhanced by 3 % though. In addition, by applying cylinder structure with appropriate design, the CCT can be modified in a large range and the white light of 8930 K has been achieved.

These simulation results provide very useful guidance for the future device fabrication. Moth-eye structure could easily enhance the extraction efficiency significantly. Due to the broadband transmission response, its CRI and CCT are very stable with varied structure dimension which is an advantage in the real fabrication. On the other hand, although the cylinder structure could only enhance the extraction efficiency by 3 %, the spectra response can be controlled by designing the structure as a thin film interferometer. Therefore, very high CRI could be achieved and CCT could be modified in a very large range under stringent processing control.

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