TiO2, SiO2, CaF2, and CaCO3: the Influence of Particles’ Concentration on Luminous Efficiency of the Conformal Geometry MCW-LEDs

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Abstract: In this research, the influence of scattering enhancement particle TiO2, SiO2, CaF2, and CaCO3 concentration, which adds to the YAG:Ce phosphor compounding, on the luminous efficiency of multichip white LEDs (MCW-LEDs) was proposed and analyzed. Firstly, the physical model of MCW-LEDs is simulated and demonstrated by using commercial LightTools 8.4 program. After that, the effect of scattering enhancement particles on the luminous efficiency is calculated and analyzed. Then, the luminous output of the 8500K W-LEDs are demonstrated convincingly by the Monte Carlo simulation and the Mie-scattering theory. The simulation results indicated that the highest luminous output could be accomplished with CaCO3 particles. The results and discussion provided a prospective approach for higher-quality manufacturing W-LEDs in the near future.

Keywords: CaCO3; CaF2; SiO2; TiO2; MCW-LEDs; lumen output

Introduction

In last decade, White LEDs (W-LEDs) had the remarkable efforts and regarded as the promising illumination method to replace the traditional lighting sources. This approach could be achieved due to their fundamental advantages, such as long lifetime, variable color, high efficiency, and low power consumption (Yu, Chung and Kim 2010, Hung and Tsao 2013). Luminous efficiency is the primary optical properties of W-LEDs, which can be improved in many previous papers (Liu et al. 2008a, Hu et al. 2011, Zheng et al. 2012, Quoc Anh et al. 2014). On the other way, several studies have proposed novel solutions to improve the luminous efficiency of LEDs by optimizing the state of the phosphor or the optical structure of PC-LEDs. It has been shown that the spatial color uniformity of PC-LEDs can be controlled by the thickness and the concentration of the phosphor (Shuai et al. 2011). Moreover, it has also been found that the location of phosphor material in the silicone layer can affect the color performance. The strong influence of the refractive indexes of the silicone matrix and the phosphor materials as well as the size of phosphor particles has been demonstrated by the color temperature of PC-LEDs (Sommer et al. 2008b).

In this paper, the effect of CaF2, SiO2 and TiO2 on the luminous efficiency of the conformal geometry MCW-LEDs is proposed and investigated. This research could be divided into three primary segments. Firstly, the physical model of 8500K W-LEDs is simulated and demonstrated by using commercial LightTools 8.1.0 program. Secondary, by adding one of scattering enhancement particles CaCO3, CaF2, SiO2 and TiO2 to the YAG:Ce phosphor compounding, the luminous efficiency of the conformal geometry MCW-LEDs is simulated, calculated and analyzed. Finally, the simulation results can be proved by using the Monte Carlo simulation and the Mie-scattering theory. In this research, the results demonstrated that the highest luminous efficiency could be accomplished with CaCO3 particles. These results are the prospective solution for higher-quality manufacturing W-LEDs in the near future.
The physical model of MCW-LEDs

The simulations were carried out using the commercial software package LightTools. The simulation comprised the setup of the conformal phosphor package (CPP) with average CCT of 8500 K. Firstly, to guarantee that the simulation results reflect precisely the impact of our considered parameters and are not biased by other factors such as LED’s wavelength, waveform, light intensity, and operating temperature, we use the real-world model of MCW-LEDs. This model possesses the best optical-thermal stability, hence, can minimize the variations caused by uninterested parameters. Secondly, to make the comparison fair, the same silicone lens and structures are used for CPP. Specifically, we set the depth, the inner and outer radius of the reflector to 2.07 mm, 8 mm and 9.85 mm, respectively. Nine LED chips are covered by either CPP or IPP, which respectively have a fixed thickness of 0.08 mm and 2.07 mm. Each blue chip has a dimension of 1.14 mm by 0.15mm, the radiant flux of 1.16 W, and the peak wavelength of 453 nm (Fig.1(a), 1(b)). Fig. 1(c) shows that the phosphor layer of CPP is coated conformally on 9 LED chips. To maintain the average CCT of 8500 K, the YAG:Ce concentration changes to the concentration of CaCO$_3$, CaF$_2$, SiO$_2$, and TiO$_2$. The refractive index of the diffusers such as CaCO$_3$, CaF$_2$, SiO$_2$ and TiO$_2$ are 1.66, 1.44, 1.47 and 2.87, respectively. The diffusers are assumed to be spherical and have radius 0.5 µm. The average radius of the phosphor particles are 7.25 µm and have a refractive index of 1.83 at all wavelengths of light. The refractive index of the silicone glue is 1.5. The diffusional particle density is varied for optimizing illumination CCT uniformity and output efficiency.

$$W_{\text{phosphor}} + W_{\text{silicone}} + W_{\text{diffuser}} = 100\% \quad (1)$$

**Results and discussion**

The commercial LightTools 8.1.0 software implements analysis of the optical properties. If the red-light is compensated enough by the scattering particles, resulting in higher lumen output (Fig. 2). Fig.2 shows luminous output values of CaCO$_3$, CaF$_2$, SiO$_2$ and TiO$_2$ case at various concentration. From the results, luminous output of MCW-LEDs by adding CaCO$_3$, CaF$_2$, SiO$_2$ increased significantly from 700 to 800 lm. However, by
adding TiO$_2$ luminous output increased and then decreased slightly. On the other word, we can say that luminous output with CaCO$_3$ particle has a considerable increase in comparison with others particle. For justifying these results, the relationship of luminous output to the diffuser weight can be formulated according to Mie-scattering theory (Shuai et al. 2011). The depletion of light is calculated by the Beer-Lambert law:

$$I = I_0 e^{-\int \mu dC_{ext}}$$  \hspace{1cm} (2)$$

Where $I$ is the transmitted light power, $I_0$ is the incident light power, $d$ is the size of the particle (mm). $L$ is the thickness of the phosphor layer thickness (mm). $N_v$ is the particle number concentration (mm$^{-3}$). $\lambda$ is the light wavelength, and $m$ is the refractive index of the medium. The following equation can express the extinction cross-section $C_{ext}$ (mm$^2$) of diffusive particles:

$$C_{ext} = \frac{2}{(\pi d / \lambda)^2} \sum_{n=1}^{\infty} (2n + 1) \text{Re}(a_n + b_n)$$  \hspace{1cm} (3)$$

The parameters $a_n$ and $b_n$ are the expansion coefficients with even symmetry and odd symmetry, respectively. These coefficients calculated by:

$$a_n(x, m) = \frac{\psi_{(m)}(x)\psi_{(x)}(x) - m\psi_{(m)}(x)\psi_{(x)}(x)}{\psi_{(m)}(x)\psi_{(x)}(x) - m\psi_{(m)}(x)\psi_{(x)}(x)}$$  \hspace{1cm} (4)$$

$$b_n(x, m) = \frac{m\psi_{(m)}(x)\psi_{(x)}(x) - \psi_{(m)}(x)\psi_{(x)}(x)}{m\psi_{(m)}(x)\psi_{(x)}(x) - \psi_{(m)}(x)\psi_{(x)}(x)}$$  \hspace{1cm} (5)$$

where $x$ is the size parameter (= kr), $m$ is the refractive index of the scattering diffusive particles, and $\psi_{(x)}$ and $\psi_{(x)}$ are the Riccati-Bessel function [20].

![Image](https://example.com/image1.png)

Figure 2. Luminous flux of W-LEDs by adding CaCO$_3$, CaF$_2$, SiO$_2$, and TiO$_2$ particles.

According to Beer-Lambert theory, if $C_{ext}$ increased, then $I$ decrease. It means extinction coefficient increases. The absorption of incident light on the measured diffuser particles can improve the sensitivity level. When the diffuser weight percentage increases, the lumen output decreases due to the excessive backward scattering in Fig.3 and Fig.4.

![Image](https://example.com/image2.png)

Figure 3. The angular scattering amplitudes of the various diffusional particles with sphere diameter = 1µm for blue light = 455 nm.

![Image](https://example.com/image3.png)

Figure 4. The angular scattering amplitudes of the different diffusional particles with sphere diameter = 1µm for yellow light = 595 nm.

**Conclusion**

In this research, the effect of CaCO$_3$, CaF$_2$, SiO$_2$, and TiO$_2$ on luminous efficiency of the 8500 K MCW-LEDs was presented, analyzed, and demonstrated. From the results, some conclusions are proposed:

1) The luminous output of MCW-LEDs by adding CaCO$_3$, CaF$_2$, SiO$_2$, particle increased significantly.

2) The luminous output of MCW-LEDs by adding TiO$_2$ increased slightly at the beginning and then decreased.

3) The lumen output of MCW-LEDs with high CCT 8500 K with CaCO$_3$ particle had a considerable increase in comparison with other particles.

This research provides essential technical implication for the selection of phosphors in WLED manufacturing and development of phosphor materials for MCW-LEDs applications. In the further works, color uniformity and color rending index of MCW-LEDs by adding CaCO$_3$, CaF$_2$, SiO$_2$, and TiO$_2$ particle into the phosphor compounding is necessary to present and demonstrate.
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