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# Simulation of Optical behavior of YAG:Ce 3+ @SiO2 phosphor used for chip scale packages WLED

--Manuscript Draft--

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| Response to Reviewers: | Dear Editors,<br>On behalf of my co-authors, we appreciate you and reviewers very much for your positive and constructive comments and suggestions. Thank you very much for your supervision of the reviewing process of our manuscript entitled “Simulation of Optical behavior of YAG:Ce3+ @SiO2 phosphor used for chip scale packages WLED” (Manuscript ID LUMIN-D-21-01164).<br><br>We also highly appreciate the reviewer’s carefulness, conscientious, and the broad knowledge on the relevant research fields, since they have given us a number of beneficial suggestions. According to the reviewer’s comments, we have studied carefully and have made the following revisions (Note: The changes in the revised manuscript had been highlighted by yellow background):<br><br>Response to the reviewer #1 : |

Comment 1: Some details in the manuscript need attention. In Figure 7, (a), (b), (d) horizontal and vertical scales are inward, and (c) horizontal and vertical scales are outward.
Response: Thank you for your careful reading of our manuscript. We have revised Figure 7 and now all the horizontal and vertical scales are inward. (see Figure 7).

Comment 2: At present, WLED has been very mature, the form of phosphorus + silicon will gradually be replaced, high-power LED and LD will become the mainstream in the future.
Response: Thank you for your constructive advice. We agree with your point that high-power LED and LD will become the mainstream in the future. For LD lighting, the cost of lasers is high and they are susceptible to environmental influences such as temperature, which will cause the light quality to decrease High-power LED mostly use glass or transparent ceramic substrates. For glass substrates, there will be diffusion problems, at high temperatures, silicon element of low temperature glass can vulnerably diffuse into phosphor particle resulting in drop in fluorescence emission intensity. This diffusion problem can be prevented if one diffusion barrier layer coated on phosphor particle surface, such as called sol-gel $Ce^{3+}$:YAG doping glass。 Therefore, our work could be also used for coated phosphor in high-power LEDs.
At mean time, our research still has some practical value to a certain extent. Firstly, YAG phosphor has low raw material prices, simple synthesis process, convenient preparation. the Chip Scale Package(CSP) technology have become one of the biggest packaging trends in recent history. It enables direct attach, can withstand higher stress, is intrinsically robust to external handling, and comes at a lower cost. It can be widely used in backlight, health inspection and car headlights, garden lighting, etc.  YAG phosphor has been used in several Samsung CSP WLED. In the CSP WLED, a blue light LED chip is usually covered with a layer of yellow fluorescent film to generate white light. It is changing the LED industry pattern, especially its supply chain. CSP LED is suitable to meet the lighting requirements such as high power and high brightness, etc. Secondly, in view of the foregoing results, we hold the opinion that this method can be extended to other coating phosphor systems and it is helpful to decrease the amount of experiments significantly. Luminescent core–shell structures appear to be very promising and are now becoming more popular in different applications. Core–shell structures show superior physical and chemical properties in comparison with their single-component counterparts, making them attractive choices for a wide range of applications not only in solid state lighting, but also in biomedicine, energy conversion, storage, and catalysis.
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Dear Editor,

We would like to submit a manuscript entitled ***"Simulation of Optical behavior of YAG:Ce3+@$SiO_2$ phosphor used for chip scale packages WLED"***, which we wish to be considered for publication in ***Journal of Luminescence*.**

Many scholars conducted experimental analysis on phosphor coating, the theoretical explanation by which phosphor coating could help improving light efficiency has not yet been studied.

In this paper, the YAG:$Ce^{3+}$ and YAG phosphor coated with $SiO_2$ layer(YAG@$SiO_2$) were chosen as the optical stimulation target. Firstly, consider the **YAG and YAG@$SiO_2$ phosphor** as spheres, the optical constants of these two phosphors were calculated based on **Mie theory**. Secondly, based on the optical constants of YAG and YAG@$SiO_2$ phosphor obtained, the luminescence performances of YAG and YAG@$SiO_2$ CSP WLED were simulated based on Monte Carlo method. Thirdly, in view of the foregoing results, we hold the opinion that this method can be extended to other coating layers and phosphor systems and it is helpful to decrease the amount of experiments significantly.

We hope that our manuscript meets the high standards of your journal. We are looking forward to your reply!

Sincerely yours,

Prof. Xinqing Su

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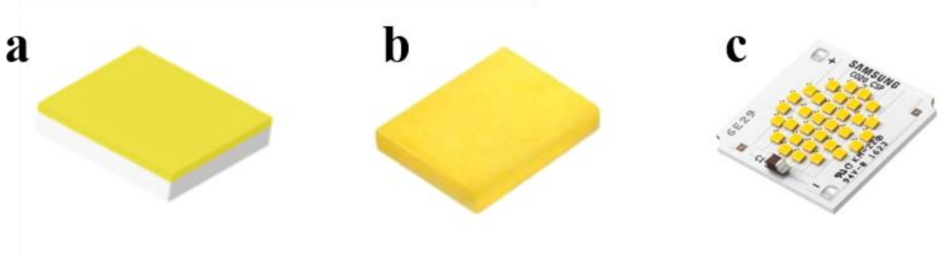


Fig. s1 Chip-scale packaged LED products (a) LM101B; (b) LH181A; (c) C020_CSP

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**Highlights**:

Many scholars conducted experimental analysis on phosphor coating, the theoretical explanation by which phosphor coating could help improving light efficiency has not yet been studied. In this paper

1. the optical constants of YAG phosphor and YAG@$SiO_2$ (YAG surface coated with nano-$SiO_2$ layer) were calculated based on Mie theory
2. the luminescence performances of YAG and YAG@$SiO_2$ CSP WLED were simulated, the results showed that the absorption coefficient of phosphor is the main concern affecting the light emission in WLED.

# Simulation of Optical behavior of YAG:$Ce^{3+}$@$SiO_2$ phosphor used for chip scale packages WLED

**Yahui Shi[1], Xinqing Su[1]*, Haitao Zhu[2], Renli Fu[1], Qinjiang He[1], Min Zhu[1] , Haidong Ren[3]***

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**Abstract:**

YAG:$Ce^{3+}$ yellow phosphor are particularly used luminescent materials to produce white light in phosphor-converted white LED (pcW-LED). Surface coating of YAG phosphor is the main concern for desired optical performance of the phosphors. Many scholars conducted various experimental analysis on the surface coating of phosphors to improve yellow emission, but the theoretical explanation by which phosphor coating could help improving light efficiency has not yet been studied. In this paper, based on Mie theory, the optical constants such as scattering coefficient, absorption coefficient and asymmetry parameter of YAG:$Ce^{3+}$ phosphor and YAG@$SiO_2$ (YAG:$Ce^{3+}$ phosphor surface coated with nano-$SiO_2$ layer) were calculated. An optical configuration of chip scale packages (CSP) WLED was constructed by coupling YAG:$Ce^{3+}$ or YAG@$SiO_2$ phosphors with a LED laser. Based on the optical parameters calculated by Mie theory, the luminescent properties of YAG:$Ce^{3+}$ and YAG@$SiO_2$ WLED were simulated by Monte Carlo method. The results showed that a thin $SiO_2$ coating layer on YAG phosphor result in an overall

increase in luminous performances compared with original YAG WLED. The absorption coefficient of phosphor is the main concern affecting the light emission in WLED. Due to the fact that YAG@$SiO_2$ possess higher $460\mu_{abs}$, it could absorb more blue light than YAG, thereby it has a 1.2% higher conversion efficiency than YAG, finally the enhanced luminous efficiency of YAG@$SiO_2$ WLED is obtained. The results obtained in this work provides a potential method in future WLED packaging designing.

**Key words:** YAG:$Ce^{3+}$ phosphor; YAG@$SiO_2$; Mie scattering; luminous efficiency.

## 1. Introduction

White lighting-emitting-diode (WLED) has been widely used in commercial solid lighting applications because of its small size, long life, energy saving, environmentally friendly and high luminous efficiency properties [1, 2]. The most appropriate method to obtain WLED is called phosphor-converted (pc-) WLED. Typically, a pc-WLED is usually fabricated by combining the blue LED chip with YAG:$Ce^{3+}$ phosphors which has acceptable color rendering and robust reliability. Traditionally, a pc-WLED package consists of LED chip, phosphors, lead frame, silicone, substrate and so on [3]. However, more packaging components in WLED package indicate higher failure possibility as well as more space occupation and more weight[4]. The chip scale package (CSP) technology is developed by covering a thin YAG fluorescent film on a blue LED chip, which could tackle this problem. The advantages of CSP WLED are the increased manufacturing efficiency [5, 6], high packing density and high luminous flux output. In the package, refractive index of silica gel (1.41) is lower than that of YAG:$Ce^{3+}$ crystal (1.84) in the thin phosphor film, therefore, more yellow light is absorbed by phosphor particle due to the total internal reflection (TIR), luminous efficiency of the CSP WLED decreases accordingly. At the same time, the refractive index difference between phosphor and silica gel leads to light scattering at the interface, which also results in the blue light reflection loss and the decrease of luminous efficiency [7]. More recently, some studies try to solve the problem by coating a dielectric layer with suitable refractive index on the phosphor. This refers to coating one or more layers of oxide material on the surface of the phosphor particles, such as $TiO_2$ [8, 9], $Al_2O_3$ [10, 11] and $SiO_2$ [12, 13]. The oxide material coating on the phosphors with matched refractive index could reduce the yellow light absorption by TIR, decrease the blue light reflection loss at the interface, in the end, improve the luminous efficiency of WLED. Among them, $SiO_2$ is widely used due to its optical transparency, tunable size [14] and low cost [15]. Many scholars conducted experimental analysis on phosphor coating, most of the studies focus on the influence of oxide layer microstructure on the luminous efficiency of WLED evaluated by photoluminescence spectra (PL spectra), but no one go deep into the light efficiency enhancement mechanism investigations. Few researchers seriously considered how the variation of light absorption and scattering of oxide layer coated phosphor affect the light extraction of WLED. Meanwhile, the optical parameters such as scattering coefficient ($\mu_{sca}$), absorption coefficient ($\mu_{abs}$) and anisotropy parameter ($\mu_{abs}$)of the coated phosphors also change as well. Actually, precise optical constants of coated phosphor are indispensable in the numerical simulation of the luminescent property of WLED. However, few research discussed about this, to the best of our knowledge.

In this paper, the YAG:$Ce^{3+}$ and YAG phosphor coated with $SiO_2$ layer(YAG@$SiO_2$) were chosen as the optical simulation target. Firstly, consider the YAG and YAG@$SiO_2$ phosphor as spheres, the optical constants of these two phosphors were calculated based on Mie theory. Secondly, based on the optical constants of YAG and YAG@$SiO_2$ phosphor obtained, the luminescence performances of YAG and YAG@$SiO_2$ CSP WLED were simulated based on Monte Carlo method.

Thirdly, in view of the foregoing results, we hold the opinion that this method can be extended to other coating layers and phosphor systems and it is helpful to decrease the amount of experiments significantly.

## 2. Description of the configuration of CSP WLED

The configuration of CSP WLED is constructed as shown in Fig. 1. In CSP LEDs, blue LED chips are mostly covered with yellow YAG fluorescent film to generate white emission (as shown in Fig.1 (e)). The YAG fluorescent film (as shown in Fig. 1(d)) is composed of phosphor particles and silica gel which are mixed in certain proportion. The optical parameters of YAG phosphor film determines the light-emitting behavior (luminous efficiency, color temperature, etc.) of the final CSP WLED. After YAG phosphor is coated by $SiO_2$ layer (as shown in Fig.1(b), the optical constants of YAG@$SiO_2$ change accordingly, which can be calculated via Mie theory.

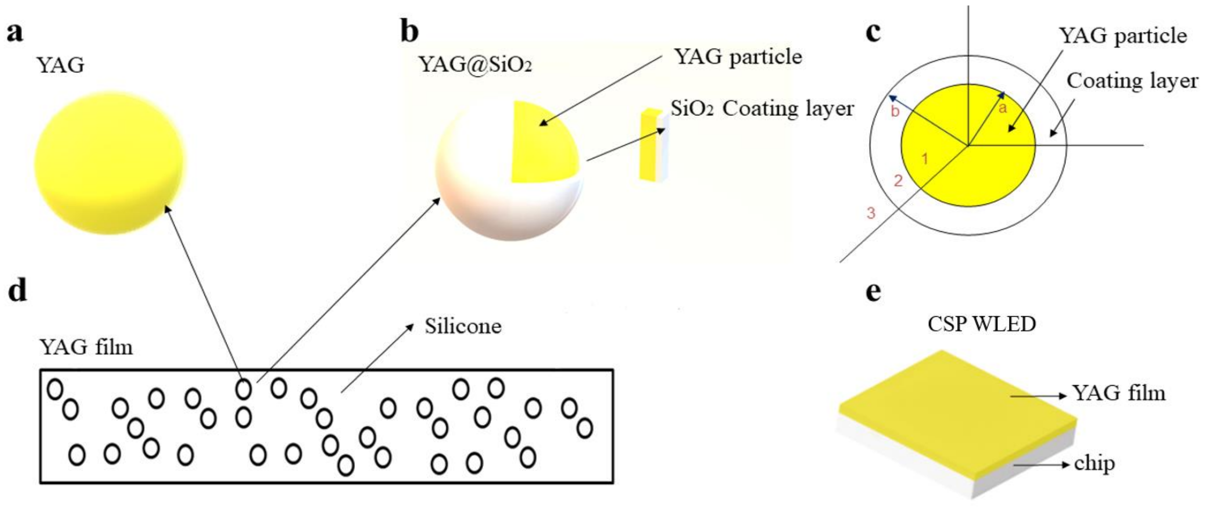


**Fig. 1 Schematic diagram of (a) YAG phosphor particle (YAG); (b) YAG phosphor coated with $SiO_2$ (YAG@$SiO_2$); (c) YAG@$SiO_2$ cross sectional view; (d) YAG film (e) CSP WLED**

We assume that spherical YAG and YAG@$SiO_2$ (YAG phosphor coated with a 10~40 nm $SiO_2$ layer) phosphor are evenly distributed in this film (as showed in Fig.1 (a) and (b)), where the yellow region is YAG phosphor and the white one is $SiO_2$ layer (as shown in Fig.1(b)). The sectional view of YAG@$SiO_2$ is shown in Fig. 1(c), in which signal 1,2,3 represent the fluorescent material (YAG), coating layer material ($SiO_2$) and silicone respectively, a and b represent the radius of YAG and YAG@$SiO_2$ phosphor, respectively.

To be convenient, we assume that, first of all, the nano-$SiO_2$ layer coated on the surface of YAG phosphor is optically transparent in the visible light range. Secondly, YAG and YAG@$SiO_2$ phosphor are ideal smooth spheres, meanwhile, $SiO_2$ layer are tightly contacted with YAG phosphor in YAG@$SiO_2$. The schematic diagram of phosphor film is shown in Fig. 1 (d). The phosphor film is consisted of phosphor particles and silicone, while the YAG phosphor particle size is set as 2 μm in this paper.

## 3. Calculation of optical constants via Mie theory

Before starting the optical simulation of WLED, the optical constants of YAG@$SiO_2$ phosphor need to be calculated via Mie theory [16]. Following is the process of the optical constants calculation. YAG phosphor can emit yellow light while being excited by blue light, thereby, 460 nm and 550 nm incident light as the light resource are chosen in the calculation. Algorithm process of optical parameters calculation is shown in Fig. 2.

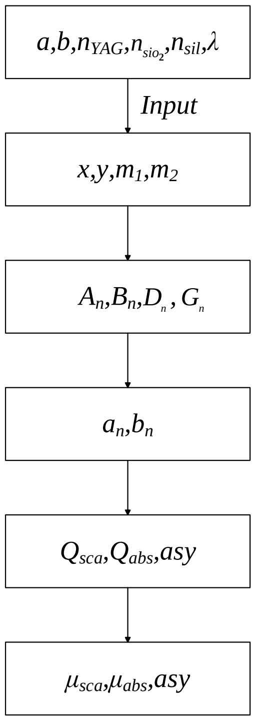


**Fig. 2 Algorithm process of optical parameters calculation**

Based on the size of YAG and YAG@$SiO_2$ phosphor ( $a$, $b$ ) , the refractive index of YAG($n_{YAG}$), $SiO_2$($n_{SiO_2}$) and silicone($n_{sil}$), the incident light wavelength in the ambient medium($\lambda$), the scattering efficiency ( $Q_{sca}$ ) , absorption efficiency ( $Q_{abs}$ ) and asymmetry parameters ( $asy$ ) of YAG or YAG@$SiO_2$ phosphor can be calculated via Mie theory. Furthermore, the absorption coefficient ($\mu_{abs}$), scattering coefficient($\mu_{sca}$) and asymmetry parameters ( $asy$ ) of YAG and YAG@$SiO_2$ phosphor can also be calculated by Mie theory. The specific calculation process is illustrated below.

According to Mie scattering theory, $x$, $y$ are the size constants, which can be calculated by equations ( 1 ) and ( 2 ) :

$$x = k \times a \tag{1}$$

$$y = k \times b \tag{2}$$

As shown in Fig. 1(c), $a$ is the radius of YAG phosphor and $b$ is the overall radius of YAG@$SiO_2$. In addition, $b$-$a$ is the coating thickness, $k$ is the wave number in the ambient medium (silicone gel) which can be described by equation (3):

$$k = \frac{2\pi n_{sil}}{\lambda} \tag{3}$$

where $\lambda$ is the incident light wavelength in the ambient medium. $n_{sil}$ is silicone gel's refractive index. $m_1$ is the refractive index of YAG phosphor relative to the ambient medium, $m_2$ is the refractive index of $SiO_2$ coating relative to the ambient medium. Silica gel is the ambient medium in LED packaging. Here the following equations (4) and (5) give the expression of $m_1$ and $m_2$.

$$m_1 = \frac{n_{YAG}}{n_{sil}} \tag{4}$$

$$m_2 = \frac{n_{SiO_2}}{n_{sil}} \tag{5}$$

YAG phosphor and $SiO_2$ both have scattering and absorption properties, so their refractive indices have a complex form:

$$n_{YAG} = n'_{YAG} - n''_{YAG} \times i \tag{6}$$

$$n_{SiO_2} = n'_{SiO_2} - n''_{SiO_2} \times i \tag{7}$$

where $n'$ and $n''$ are the real and imaginary refractive indices of the phosphor particle, respectively. Tab. 1 shows the refractive indices of YAG and $SiO_2$ which are used in calculation.

**Table 1** Refractive indices of YAG and $SiO_2$

| Component | $n'$ | $n''$ |
|---|---|---|
| $SiO_2$ coating [17] | 460 nm, $n'_{SiO_2}$ = 1.484 | $n''_{SiO_2}$ = 4.00E-07 |
| | 550 nm, $n'_{SiO_2}$ = 1.479 | $n''_{SiO_2}$ = 4.00E-07 |
| YAG [18] | 460 nm, $n'_{YAG}$ = 1.851 | $n''_{YAG}$ = 5.12E-04 |
| | 550 nm, $n'_{YAG}$ = 1.839 | $n''_{YAG}$ = 1.31E-05 |

Here the following equations (8) to (11) give the expression for $A_n$, $B_n$, $D_n$ *and* $m$, where $\psi_n$

and $\chi_n$ are Bessel functions, $m$ is the refractive index with respect to the ambient medium, $D_n$ is the logarithmic derivative of $\psi_n$.

$$A_n = \psi_n(m_2x)\frac{mD_n(m_1x) - D_n(m_2x)}{mD_n(m_1x)\chi_n(m_2x) - \chi_n^{'}(m_2x)} \tag{8}$$

$$B_n = \psi_n(m_2x)\frac{D_n(m_1x)/m - D_n(m_2x)}{D_n(m_1x)\chi_n(m_2x) - \chi_n^{'}(m_2x)} \tag{9}$$

$$m = \frac{m_2}{m_1} \tag{10}$$

$$D_n = \frac{\psi'_n(mx)}{\psi_n(mx)} \tag{11}$$

Here the following equations (12) and (13) give the expression for $D_n$ and $G_n$.

$$\tilde{D}_n = \frac{D_n(m_2y) - \dfrac{A_n\chi_n^{'}(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{A_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{12}$$

$$\tilde{G}_n = \frac{D_n(m_2y) - \dfrac{B_n\chi_n^{'}(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{B_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{13}$$

In Mie scattering theory, $a_n$ and $b_n$ are the Mie expansion scattering coefficients. They could be expressed by equations (14) and (15):

$$a_n = \frac{(\tilde{D}_n/m_2 + n/y)\psi_n(y) - \psi_{n-1}(y)}{(\tilde{D}_n/m_2 + n/y)\xi_n(y) - \xi_{n-1}(y)} \tag{14}$$

$$b_n = \frac{(m_2\tilde{G}_n + n/y)\psi_n(y) - \psi_{n-1}(y)}{(m_2\tilde{G}_n + n/y)\xi_n(y) - \xi_{n-1}(y)} \tag{15}$$

where $\xi_n$ is Hankel functions of second kind.

According to Mie scattering theory, the extinction efficiency $Q_{ext}$, the scattering efficiency $Q_{sca}$, the absorption efficiency $Q_{abs}$, and the asymmetry parameter *asy* of optical medium are calculated according to equations (16) to (19) [19].

$$Q_{sca} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)\left(\left|a_n\right|^2+\left|b_n\right|^2\right) \tag{16}$$

$$Q_{ext} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)Re\left(a_n+b_n\right) \tag{17}$$

$$Q_{abs}=Q_{ext}-Q_{sca} \tag{18}$$

$$asy=\frac{4}{x^2}\left\{\sum_{n=1}^{\infty}Re(a_n a_{(n+1)}^{*}+b_n b_{(n+1)}^{*})\right\}/Q_{sca} \tag{19}$$

Among them, $R_e$ represents the real part of the complex number, * represents the transpose.

Based on the results of $Q_{sca}$, and $Q_{abs}$, the absorption coefficient $(\mu_{abs})$ *and* scattering coefficient $(\mu_{sca})$ of YAG and YAG@$SiO_2$ are calculated according to equations (20) and (21)[20].

$$\mu_{abs}=Q_{abs}Av_f\cdot\left(1/V\right)=3Q_{abs}v_f/4b \tag{20}$$

$$\mu_{sca}=Q_{sca}Av_f\cdot\left(1/V\right)=3Q_{sca}v_f/4b \tag{21}$$

where $A$ is the geometrical cross area of the phosphor particle, $V$ is the volume of the particle , $v_f$ is the volume fraction of YAG or YAG@$SiO_2$. For YAG@$SiO_2$, $v_f$ is described by equation (22):

$$v_f=\frac{m_{YAG}/\rho_{YAG}+m_{SiO_2}/\rho_{SiO_2}}{m_{YAG}/\rho_{YAG}+m_{SiO_2}/\rho_{SiO_2}+m_{sil}/\rho_{sil}} \tag{22}$$

$m_{YAG}$ is the mass of YAG phosphor, $m_{SiO_2}$ is the mass of $SiO_2$, $m_{sil}$ is the mass of silica gel, $\rho_{YAG}$ is the density of YAG phosphor, $\rho_{SiO_2}$ is the density of $SiO_2$ and $\rho_{sil}$ is the density of silica gel. In this calculation, $\rho_{YAG}$ , $\rho_{SiO_2}$ and $\rho_{sil}$ are set as 4.6, 2.2 and 1.1 g/cm$^3$, respectively. In practical applications, mass fraction of YAG phosphor ($w_f$) in phosphor film is more commonly used instead of the volume fraction of phosphor ($v_f$), it is expressed as following:

$$w_f = \frac{m_{YAG} + m_{SiO_2}}{m_{YAG} + m_{SiO_2} + m_{Sil}} \quad (23)$$

The absorption coefficient ($\mu_{abs}$), scattering coefficient ($\mu_{sca}$) and asymmetry parameter ($asy$) of the phosphor film affect the light absorption and scattering, therefore, show great influence on the light extraction and the final luminous efficiency of WLED. Concentration of YAG phosphors and a, b values are the main factors that affect the optical constants $\mu_{abs}$ , $\mu_{sca}$ and $asy$ of the final fluorescent film. The influence of coating thickness (b-a), mass fraction of the phosphor ($w_f$) and incident light wavelength (λ) on $\mu_{abs}$ , $\mu_{sca}$ and $asy$ of phosphor film are discussed through Mie scattering theory calculation. Generally, 460nm blue light excites YAG phosphor and generates yellow light with a dominant wavelength of 550nm. For simplicity , 460 $\mu_{abs}$ and 550 $\mu_{abs}$ denote the absorption coefficient of phosphors excited by 460nm and 560nm incident light, respectively. 460 $\mu_{sca}$ and 550 $\mu_{sca}$ denote the scattering coefficient of phosphors excited by 460nm and 560nm incident light, respectively.

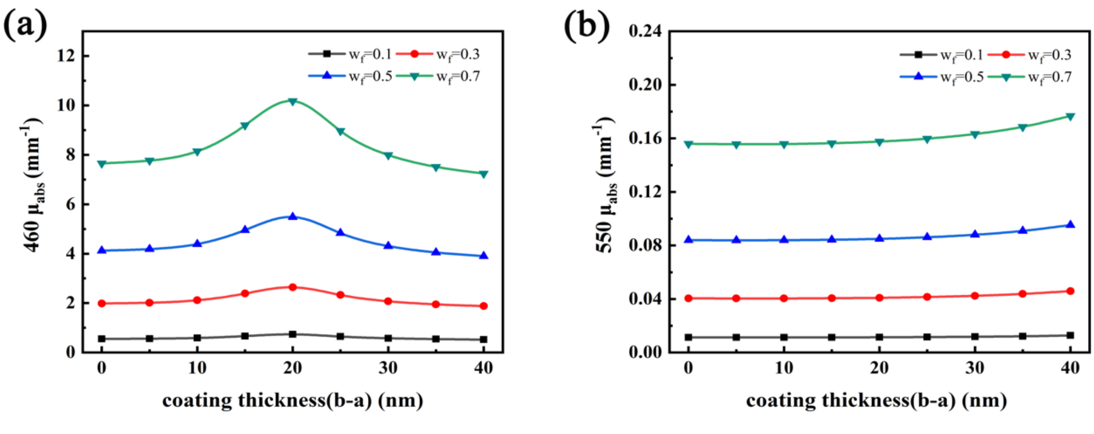


**Fig. 3 $\mu_{abs}$of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig.3 (a), 460$\mu_{abs}$ increased as the thickness of $SiO_2$ layer increased from 0 to 20 nm, and then decreased when continue increasing the thickness to 40 nm. It is obviously noticed that

$460\mu_{abs}$ reached the highest value when the phosphor coating is 20nm. Compared with pristine phosphor , after being coated with nano-$SiO_2$ layer, the photons mainly transmit the $SiO_2$ layer via increasing the absorption of blue light due to the low refractive index of $SiO_2$ and then get to the phosphor surface , therefore, the effective excitation absorption of the phosphor via the $SiO_2$ layer occurred [9]. Based on Lambert-Beer's law, the transmitted light through a layer of coating is inversely proportional to the thickness of coating material. Although the coating layer can decrease the reflectance (which enhances the luminescence properties), while the quantity of light escaping from phosphor is reduced in much thicker layer [13]. Therefore, in our research, when the coating thickness is 20nm, the absorption of 460nm blue light by YAG@ $SiO_2$ find the maximum value. Our calculation is entirely consistent with previous reports [13,21].

The incident light absorption coefficient $460\mu_{abs}$ and $550\mu_{abs}$ are not in the same order of magnitude as shown in Fig.3. $550\mu_{abs}$ is much smaller than $460\mu_{abs}$. Meanwhile, as shown in Fig.3 (b), for 550nm incident light, the thickness of the $SiO_2$ coating layers had little influence on the absorption coefficient of YAG phosphor film. All these are due to the fact that YAG phosphor crystals show quite different absorption coefficients while excited by blue or yellow light [22, 23], for blue light the absorption coefficient is 3-8$mm^{-1}$, however it is only 0.1-0.5$mm^{-1}$ for yellow light. Our calculation is in accordance with the experimental results.

While considering about the influence of mass fraction of the phosphor ( $w_f$ ) on $460\mu_{abs}$ or $550\mu_{abs}$, as $w_f$ increased from 0.1 to 0.7, there are more phosphor particles in the fluorescent film, the absorption of incident light increased, thus, $460\mu_{abs}$ or $550\mu_{abs}$ increased accordingly.

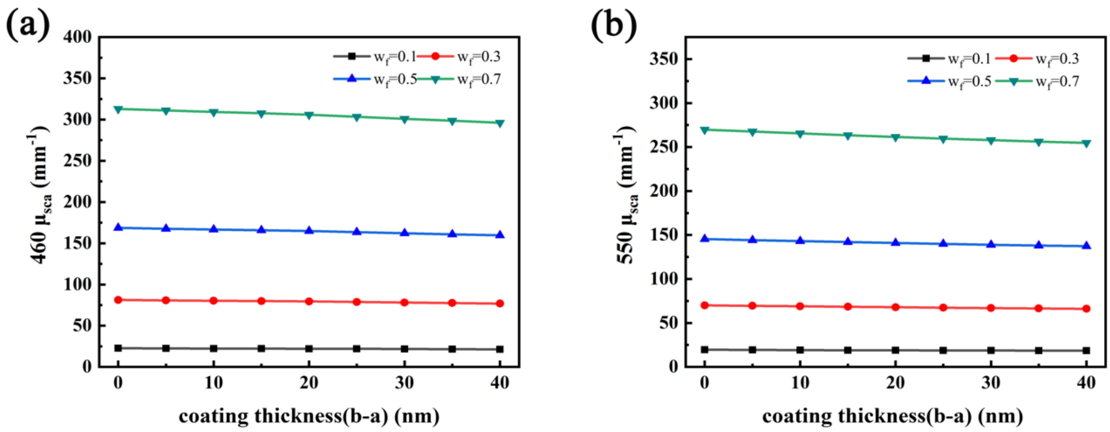


**Fig.4 $\mu_{sca}$ of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig. 4, when the thickness of the $SiO_2$ coating layer increased, 460 $\mu_{sca}$ and 550$\mu_{sca}$ of YAG@$SiO_2$ both slightly decreased, illustrated that less light energy is lost by scattering and more energy can be used for illumination by coating thicker $SiO_2$ layer. It is noting that using phosphors with smaller scattering coefficient could be a way to suppress the scattering loss. The results indicated that coating of $SiO_2$ suppressed the scattering loss in a certain extent [19]. While increase $w_f$ of phosphor from 0.1 to 0.7, more light was scattered because there is more phosphor in the fluorescent film. Comparing the results in Fig.4 (a) and (b), it is found that the variation of $\mu_{sca}$ is very small when the incident light changes from blue light to yellow light. This indicates that the scattering property of coated phosphors are similar with uncoated one for different light, the big difference of absorption property between coated phosphor and uncoated one might be the main reason that affect the light extraction and luminous efficiency of WLED.

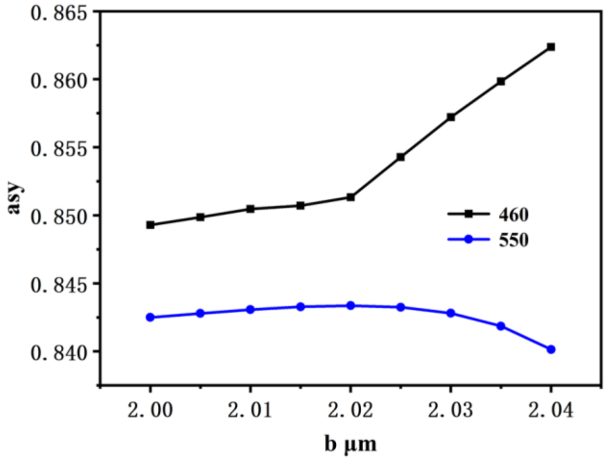


**Fig.5 Asymmetry parameter *asy* of phosphor film**

As shown in Fig.5, while excited by 460 nm or 550 nm incident light, *asy* of YAG and YAG@$SiO_2$ phosphor were positive, which meant under this condition, the number of forward scattered lights were greater than the number of backscattered lights [20]. While the coating thickness increased to 20nm, *asy* (460 nm or 550 nm excitation) increased a little, indicated the increasing of forward scattering. When coating thickness exceeded 20 nm, *asy* of YAG@$SiO_2$ had opposite trends while excited by 460 nm blue light or 550 nm yellow light. The increase of $asy_{460}$ indicated that the scattered light concentrated in smaller forward scattering angle, which resulted in an increase in the number of forward scattered light. Reversely, the decrease of $asy_{550}$ meant that more light was backscattered, absorbed and converted into heat loss. Herein, the backscattering loss of the emission from phosphor particles decreased the external quantum efficiency of the white LED [24]. If there are more forward scattered light existed in the packaged WLED, the luminous efficiency is improved as a result. The results in Fig.5 shows that the value of $asy_{550}$ and $asy_{460}$ is very close. When coating thickness changes, there is no great variation in *asy*. However, based on the previous results, it is clear that scattering property of phosphors is not the main reason for light extraction in packaged WLED. The tiny difference between $asy_{550}$ and $asy_{460}$ almost have no effect on light extraction in packaged WLED.

## 4. Optical simulation of CSP WLED

In most commercial optical software such as Light Tools and Trace Pro, the phosphor scattering is normally treated as Mie scattering to bring about the optical simulation of white LED packaging. The precise optical constants calculation via Mie theory could afford necessary supports for the optical simulation in LED packaging design.

Depend on these obtained optical constants $\mu_{abs}$ , $\mu_{sca}$ and $asy$, we carried out the photoluminescence property simulation for YAG and YAG@$SiO_2$ WLED by Monte Carlo ray tracing method. The configuration of CSP WLED is given in Fig.6. The phosphor film is coated on the surface of the flip chip LED. The CSP chip is a 1 W blue LED chip or yellow LED chip (SAMSUNG LM101B) with dimension of 1mm×1mm×H mm, while H denotes the phosphor film thickness. The receiving surface (Receiver F) is assumed as a perfect absorber which collects blue light emitted from the blue LED chip and yellow light emitted from YAG or YAG@$SiO_2$ phosphor. To simplify the simulation, the radius of YAG particles is fixed at 2μm, coating thickness of YAG@$SiO_2$ is set at 20nm, mass fraction of the phosphor ($w_f$) in phosphor film is set at 0.7.

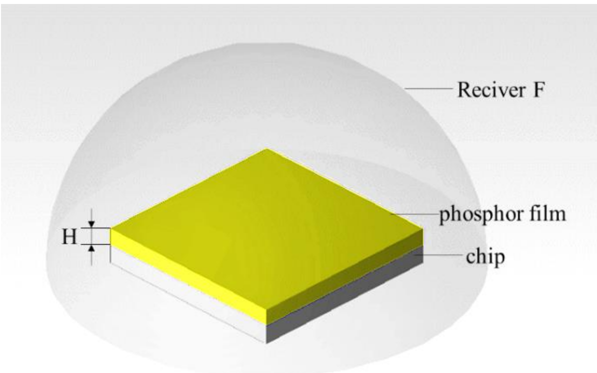

**Fig.6** Configuration **of Chip-Scale-Packaged (CSP) WLED**

Generally, the most important thing in WLED packaging is the absorption and scattering properties of YAG phosphor for blue light emit from the chip and the yellow light emit from YAG phosphor itself. When the phosphor is excited by 460 nm blue light, the transmitted light is divided into two parts, unchanged blue light and converted yellow light. For 550 nm yellow light excitation, since no converted light is emitted from the phosphor film, the transmitted light is sorted as the yellow light. In this simulation, two 1W color LEDs with peak wavelength of 460 and 550nm are used as the light sources, coating thickness of YAG@$SiO_2$ is fixed at 20nm and the thickness of the phosphor film changes from 0.05 to 0.30 mm. The influence of the phosphor film thickness on light emission of CSP WLED was investigated and the results are shown in Fig.7. For the sake of simplicity, the transmittance for the unconverted blue light emit from blue LED and converted yellow light emit from phosphor are denoted as $\eta_{460\mathrm{BT}}$ and $\eta_{460YT}$. The transmittance of yellow light emit from yellow LED are denoted as $\eta_{550\mathrm{YT}}$. The total yellow light emits from phosphor excited by yellow LED are denoted as $\eta_{550\mathrm{Y}}$. The subscript of these signals, such as 460 and 550 indicate the excitation wavelength.

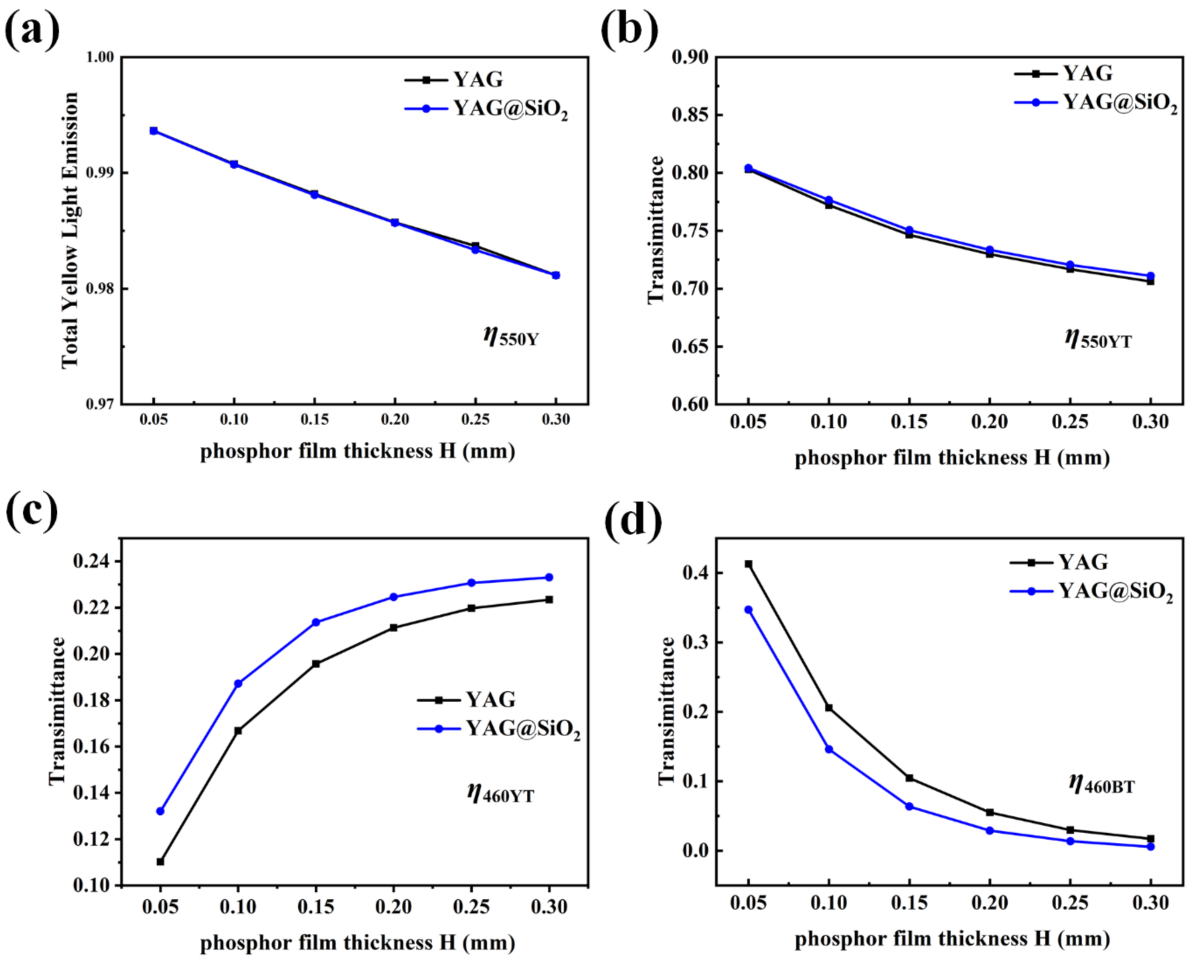


**Fig. 7** Simulation results of **(a)** Total yellow light emission from phosphor, the transmittance of YAG and YAG@$SiO_2$ phosphors for (b) yellow light emit from yellow LED (c) converted light emit from phosphor excited by blue light and (d) blue light emit from blue LED

As shown in Fig. 7 (a), when the phosphor is excited by 550nm yellow light, the total amount of yellow light scattered from YAG@$SiO_2$ phosphor is almost consistent with it from YAG phosphor. It is because $SiO_2$ almost has no absorption in the visible light range, hence, the absorption of yellow light by $SiO_2$ is negligible as shown in Fig. 7 (a). As seen from Table 1, the absorption coefficients of $SiO_2$ at 460nm and 550nm are basically the same, therefore, the absorption of 460nm blue light by the coated 20nm $SiO_2$ layer is also negligible.

As seen from the results of Fig.5, 550*asy* increase slightly while YAG phosphor was coated by 20nm $SiO_2$, indicates that under yellow light illumination, more of the light is forward scattered compared with pristine YAG phosphor. Therefore, as seen from Fig.7(b), $\eta_{550YT}$ of YAG@$SiO_2$ is slightly higher than that of YAG phosphor. Based on Lambert-Beer's law, more light is absorbed when the thickness of the phosphor film H increased from 0.05 to 0.3mm, therefore, $\eta_{550YT}$ of YAG and YAG@$SiO_2$ decreased as a result.

Fig. 7(c) and (d) show us the transmittance for the converted yellow light ($\eta_{460YT}$) and the unconverted blue light ($\eta_{460BT}$) excited by blue LED. It shows that $\eta_{460YT}$ increase but $\eta_{460BT}$ decrease while the phosphor film thickness increase. This is in accordance with the result of Lambert-Beer's law，while more blue light could be absorbed by phosphors as the phosphor film is thicker, therefore, less unconverted blue light but more converted yellow light emit out. When the phosphor film thickness is the same, $\eta_{460YT}$ of YAG@$SiO_2$ is greater than that of YAG. This is due to the fact that YAG@$SiO_2$ possess higher $460\mu_{abs}$ (see Fig.4(a)), hence more blue light is absorbed by YAG@$SiO_2$ compared with YAG, accordingly more light is converted into yellow light. The simulation results indicate that a thin $SiO_2$ layer does help to increase the yellow light emission, as many earlier scholars reported. [13,21]

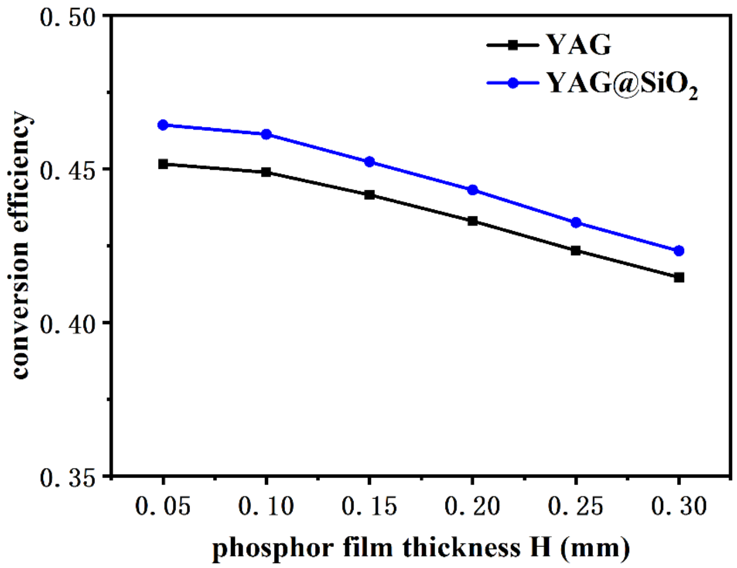


**Fig. 8 Conversion efficiency of phosphor**

Fig. 8 shows the conversion efficiency of YAG and YAG@$SiO_2$ excited by blue LED. As the thickness of the phosphor film increases, the conversion efficiency of phosphor gradually decreases, it might due to the fact that when the film is too thick or the phosphor concentration is too high, the oversaturated phosphor causes more converted light to be back reflected [19], and less light to be forward reflected. This might cause multiple reflection of the converted light between the phosphor layer and the chip. The multiple reflection result in the high absorption of converted light and decrease of luminous efficiency. However, YAG@$SiO_2$ has a 1.2% higher conversion efficiency than YAG, which implies that phosphor coating might be an effective way to improve the light efficiency.

In order to generate white light, the luminescence efficiency and true color map of the CSP WLED with different YAG film thickness ( H ) is simulated. As the thickness of the YAG fluorescent film increases, the luminous efficacy and color temperature of blue LED excited WLED gradually increase. When H is 0.3mm, the luminous efficiency gradually reaches saturation. When H is 0.2mm, the fabricated CSP LED possess a cold white light emission with a CCT of 10066K, color coordinates of (0.2851, 0.2786)（as shown in Fig.11(b)）and a luminous efficacy up to 130.3 lm/W (as shown in Fig.9).

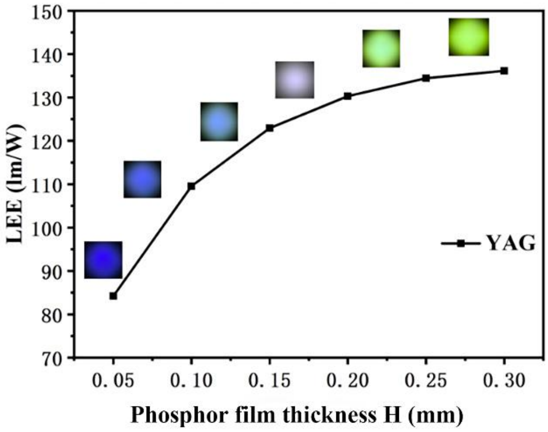


**Fig. 9 Influence of YAG fluorescent film thickness on luminous efficiency of YAG WLED**

The fluorescent film thickness (H) is fixed at 0.2mm, the influence of $SiO_2$ coating thickness on the luminous efficiency (LEE) and Correlate Color Temperature (CCT) of CSP WLED are shown in Fig.10. With the increasing of $SiO_2$ coating thickness, LEE of CSP WLED firstly increase and then decrease. When the coating thickness is 20nm, the luminous efficacy reached the maximum value 138.92 lm/W. This might due to the fact that $460\mu_{abs}$ of YAG@$SiO_2$ phosphor reaches the highest value while the $SiO_2$ coating thickness is 20 nm. Under this condition, more blue light emitted from the chip could be absorbed by YAG@$SiO_2$ phosphor film. More absorption of blue light by the YAG@$SiO_2$ phosphor, more emission of yellow light, therefore enhanced LEE is obtained.

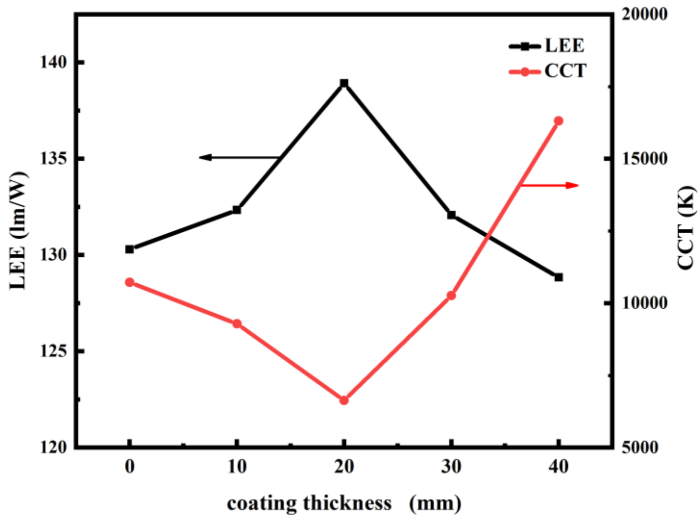


**Fig.10 Influence of coating thickness on LEE and CCT of CSP WLED**

Meanwhile, CCT of YAG@$SiO_2$ WLED decreases when the thickness of $SiO_2$ coating layer increases from 0 to 20 nm. When the thickness of the $SiO_2$ coating layer is over 20 nm, the color temperature of YAG@$SiO_2$ WLED increases sharply. Low color temperature WLED is prefer under working condition. It is found that proper $SiO_2$ layer thickness endowing YAG@$SiO_2$ with more absorption of blue light and high output of yellow light, therefore significantly enhance the LEE and decrease the CCT of WLED. The highest value of LEE, 138.92 lm/W, the lowest CCT, 6667K, are achieved at a $SiO_2$ layer thickness of 20nm. The simulation results above show that proper $SiO_2$ coating on phosphors is responsible for the enhanced luminous efficacy and lower color temperature of CSP WLED, which is in accordance with the former reports. [21]

Using Monte Carlo method, the quality of white light emission from the YAG and YAG@$SiO_2$ WLED was evaluated via CIE chromaticity diagram and Luminous flux figure (as shown in Fig.11). The results are listed in Table 2.

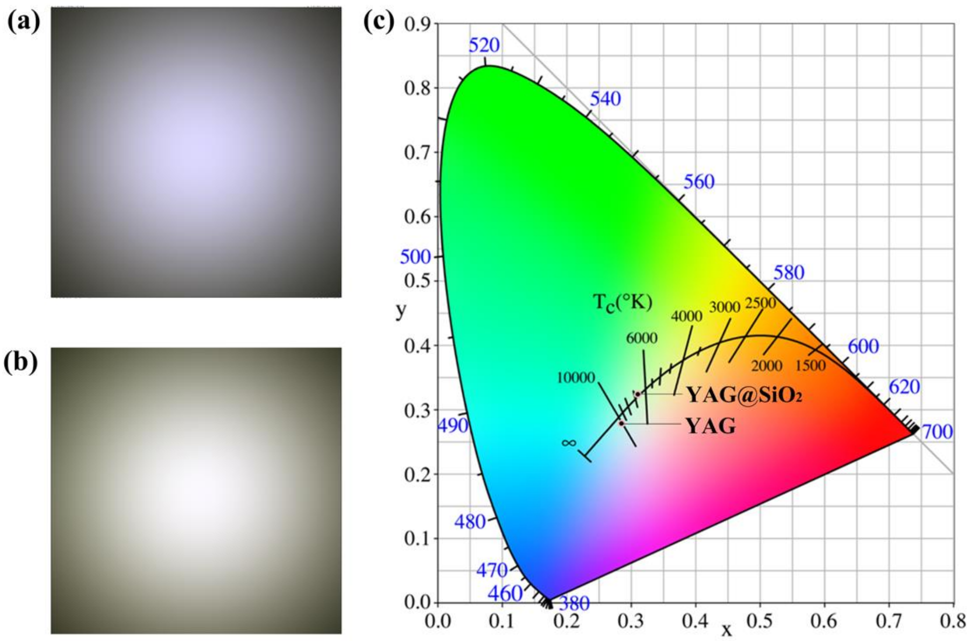


**Fig. 11 (a) Luminous flux figure of YAG WLED; (b)Luminous flux figure of YAG@$SiO_2$WLED; (c) Chromaticity color coordinates of YAG and YAG@$SiO_2$ upon excitation at 460 nm**

**Table. 2 Optical properties of YAG and YAG@$SiO_2$ WLEDs Simulated by Monta Carlo Ray Tracing method**

| Phosphor | LEE （lm/W） | CCT (K) | CIE (x, y) | Fluorescence conversion efficiency |
|---|---|---|---|---|
| YAG | 132.11 | 10066 | (0.2851,0.2786) | 0.4299 |
| YAG@$SiO_2$ | 138.92 | 6637 | (0.3110,0.3244) | 0.4392 |

When the thickness of fluorescent film is 0.2 mm, $SiO_2$ coating layer is 20 nm, YAG@$SiO_2$ WLED shows a light efficiency of 138.92 lm/W, a color temperature of 6637K, and a color coordinate of (0.3110, 0.3244), as shown in Tab.2. Compared with original YAG WLED, higher LEE and lower CCT is achieved in YAG@$SiO_2$ WLED, which is resulted from enhanced forward scattering and stronger blue light absorption. Meanwhile, the color coordinates of YAG@$SiO_2$ WLED is closer to the theoretical white point of (0.33, 0.33). This result shows that an ideal white color is almost achieved in YAG@$SiO_2$ under 460nm blue LED excitation. Meanwhile, proper $SiO_2$

thin layer coating on YAG significantly enhanced LEE and CCT of WLED, and a good cold white light emission is achieved.

Our simulation gives a theoretical explanation about the reason why proper coating thickness on YAG phosphor endows the CSP WLED with higher luminous efficacy and lower color temperature, hence better luminescence properties.

## 5. Conclusions

Optical configuration of chip scale packages WLEDs are established by coating YAG or YAG@$SiO_2$ phosphor film directly on the chip surface. In order to ensure the correct simulation of luminescence properties of the CSP white LED, the specific optical constants including the absorption coefficient $\mu_{abs}$, scattering coefficient $\mu_{sca}$, and anisotropy factor $asy$ of YAG and YAG@$SiO_2$ are calculated based on Mie scattering theory. The dependency of coating thickness of $SiO_2$ layer and phosphor mass fraction $w_f$ on optical constants $\mu_{abs}, \mu_{sca}$ and $asy$ are investigated. It shows that when the coating thickness is 20 nm, the absorption coefficient increases the most, which is conducive to increase the absorption of blue light, enhance the yellow light emission and eventually improve the luminescence property. The decrease in scattering coefficient is also conducive to the improvement of luminous efficiency. Numerical results show that Mie theory is effective in predicting the changing tendencies of the optical constants as the mass fraction of phosphor or the coating thickness changes. It makes Mie theory a suitable tool in WLED packaging design. Two color LEDs are used as light sources to simulate the light extraction of YAG and YAG@$SiO_2$ WLED via Monte Carlo ray tracing method. It implies that $SiO_2$ coating mainly result in the enhanced absorption of blue light and yellow light converting, hence the higher conversion efficiency for YAG@$SiO_2$. As the thickness of the fluorescent film is 0.2 mm, with 2 μm YAG@$SiO_2$ coated by 20 nm $SiO_2$ layer in it, our WLED gives a light efficiency of 138 lm/W, a color temperature of 6637 K, and a color coordinate of (0.3110, 0.3244), The light conversion efficiency after coating is increased by 1.2% compared with that before coating.

The simulation of photoluminescence property of YAG@$SiO_2$ WLED can be adapted to various coated phosphors WLED systems, the color quality can be easily tuned by changing the coating thickness, the phosphor film thickness or the mass fraction of phosphor, which have potential use in the future WLED packaging designing.

## Acknowledgment

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# Simulation of Optical behavior of $YAG:Ce^{3+}@SiO_2$ phosphor used for chip scale packages WLED

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**Abstract**

$YAG:Ce^{3+}$ yellow phosphor are particularly used luminescent materials to produce white light in phosphor-converted white LED (pc-WLED). Surface coating of YAG phosphor is the main concern for desired optical performance of the phosphors. Many scholars conducted various experimental analysis on the surface coating of phosphors to improve yellow emission, but the theoretical explanation by which phosphor coating could help improving light efficiency has not yet been studied. In this paper, based on Mie theory, the optical constants such as scattering coefficient, absorption coefficient and asymmetry parameter of $YAG:Ce^{3+}$ phosphor and $YAG@SiO_2$ ($YAG:Ce^{3+}$ phosphor surface coated with nano-$SiO_2$ layer) were calculated. An optical configuration of chip scale packages (CSP) WLED was constructed by coupling $YAG:Ce^{3+}$ or $YAG@SiO_2$ phosphors with a LED laser. Based on the optical parameters calculated by Mie theory, the luminescent properties of $YAG:Ce^{3+}$ and $YAG@SiO_2$ WLED were simulated by Monte Carlo method. The results showed that a thin $SiO_2$ coating layer on YAG phosphor result in an overall increase in luminous performances compared with original YAG WLED. The absorption coefficient of phosphor is the main concern affecting the light

emission in WLED. Due to the fact that YAG@$SiO_2$ possess higher $460\mu_{abs}$, it could absorb more blue light than YAG, thereby it has a 1.2% higher conversion efficiency than YAG, finally the enhanced luminous efficiency of YAG@$SiO_2$ WLED is obtained. The results obtained in this work provides a potential method in future WLED packaging designing.

## 1. Introduction

White lighting-emitting-diode (WLED) has been widely used in commercial solid lighting applications because of its small size, long life, energy saving, environmentally friendly and high luminous efficiency properties [1, 2]. The most appropriate method to obtain WLED is called phosphor-converted (pc-) WLED. Typically, a pc-WLED is usually fabricated by combining the blue LED chip with YAG:$Ce^{3+}$ phosphors which has acceptable color rendering and robust reliability. Traditionally, a pc-WLED package consists of LED chip, phosphors, lead frame, silicone, substrate and so on [3]. However, more packaging components in WLED package indicate higher failure possibility as well as more space occupation and more weight[4]. The chip scale package (CSP) technology is developed by covering a thin YAG fluorescent film on a blue LED chip, which could tackle this problem. The advantages of CSP WLED are the increased manufacturing efficiency [5, 6], high packing density and high luminous flux output. In the package, refractive index of silica gel (1.41) is lower than that of YAG:$Ce^{3+}$ crystal (1.84) in the thin phosphor film, therefore, more yellow light is absorbed by phosphor particle due to the total internal reflection (TIR), luminous efficiency of the CSP WLED decreases accordingly. At the same time, the refractive index difference between phosphor and silica gel leads to light scattering at the interface, which also results in the blue light reflection loss and the decrease of luminous efficiency [7]. More recently, some studies try to solve the problem by coating a dielectric layer with suitable refractive index on the phosphor. This refers to coating one or more layers of oxide material on the surface of the phosphor particles, such as $TiO_2$ [8, 9], $Al_2O_3$ [10, 11] and $SiO_2$ [12, 13]. The oxide material coating on the phosphors with matched refractive index could reduce the yellow light absorption by TIR, decrease the blue light reflection loss at the interface, in the end, improve the luminous efficiency of WLED. Among them, $SiO_2$ is widely used due to its optical transparency, tunable size [14] and low cost [15]. It has been have concluded that $SiO_2$-coated YAG phosphor limits the thermal quenching properties[16, 17]. Therefore, YAG phosphor coated with $SiO_2$ layer(YAG@$SiO_2$) could be considered as a good candidate for white light-emitting diode applications[18]. Many scholars conducted experimental analysis on phosphor coating, most of the studies focus on the influence of oxide layer microstructure on the luminous efficiency of WLED evaluated by photoluminescence spectra (PL spectra), but no one go deep into the light efficiency enhancement mechanism investigations. Few researchers seriously considered how the variation of light absorption and scattering of oxide layer coated phosphor affect the light extraction of WLED. Meanwhile, the optical parameters such as scattering coefficient ($\mu_{sca}$), absorption coefficient ($\mu_{abs}$) and anisotropy parameter ($\mu_{abs}$)of the coated phosphors also change as well. Actually, precise optical constants of coated phosphor are indispensable in the numerical simulation of the luminescent property of WLED. However, few research discussed about this, to the best of our knowledge.

In this paper, the YAG:$Ce^{3+}$ and YAG@$SiO_2$ were chosen as the optical simulation target. Firstly, consider the YAG and YAG@$SiO_2$ phosphor as spheres, the optical constants of these two phosphors were calculated based on Mie theory. Secondly, based on the optical constants of YAG and YAG@$SiO_2$ phosphor obtained, the luminescence performances of YAG and YAG@$SiO_2$ CSP WLED were simulated based on Monte Carlo method. Thirdly, in view of the foregoing results, we hold the opinion that this method can be extended to other coating layers and phosphor systems and it is helpful to decrease the amount of experiments significantly.

## 2. Description of the configuration of CSP-packaged WLED

The configuration of CSP-packaged WLED is constructed as shown in Fig. 1. In CSP LEDs, blue LED chips are mostly covered with yellow YAG fluorescent film to generate white emission (as shown in Fig.1 (e)). The YAG fluorescent film (as shown in Fig. 1(d)) is composed of phosphor particles and silica gel which are mixed in certain proportion. The optical parameters of YAG phosphor film determines the light-emitting behavior (luminous efficiency, color temperature, etc.) of the final CSP WLED. After YAG phosphor is coated by $SiO_2$ layer (as shown in Fig.1(b), the optical constants of YAG@$SiO_2$ change accordingly, which can be calculated via Mie theory.

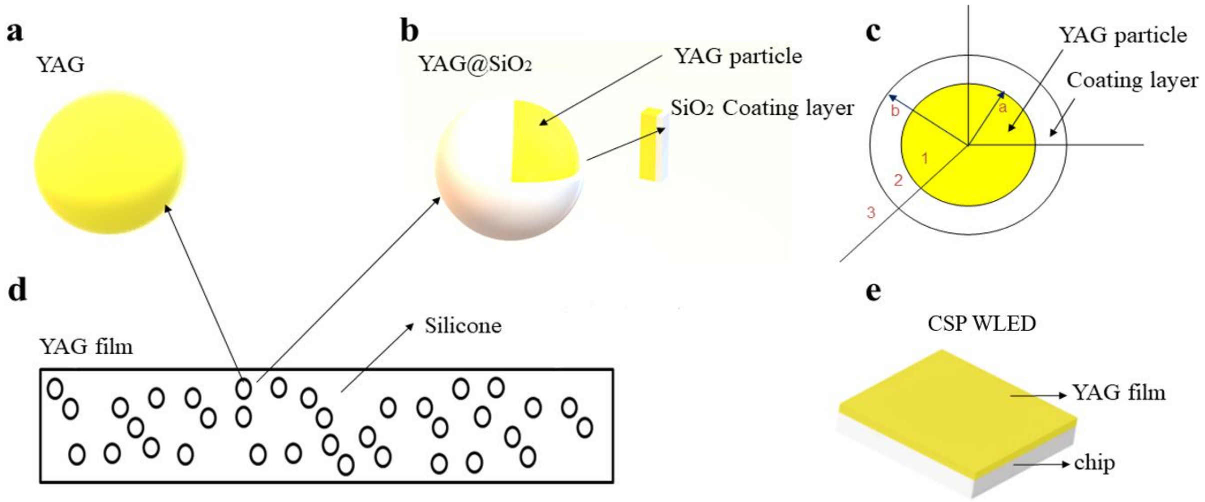


**Fig. 1 Schematic diagram of (a) YAG phosphor particle (YAG); (b) YAG phosphor coated with $SiO_2$ (YAG@$SiO_2$); (c) YAG@$SiO_2$ cross sectional view; (d) YAG film (e) CSP WLED**

We assume that spherical YAG and YAG@$SiO_2$ (YAG phosphor coated with a 10~40 nm $SiO_2$ layer) phosphor are evenly distributed in this film (as showed in Fig.1 (a) and (b)), where the yellow region is YAG phosphor and the white one is $SiO_2$ layer (as shown in Fig.1(b)). The sectional view of YAG@$SiO_2$ is shown in Fig. 1(c), in which signal 1,2,3 represent the fluorescent material (YAG), coating layer material ($SiO_2$) and silicone respectively, a and b represent the radius of YAG and YAG@$SiO_2$ phosphor, respectively.

To be convenient, we assume that, first of all, the nano-$SiO_2$ layer coated on the surface of YAG phosphor is optically transparent in the visible light range. Secondly, YAG and YAG@$SiO_2$ phosphor are ideal smooth spheres, meanwhile, $SiO_2$ layer are tightly contacted with YAG phosphor in YAG@$SiO_2$. The schematic diagram of phosphor film is shown in Fig. 1 (d). The phosphor film is consisted of phosphor particles and silicone, while the YAG phosphor particle size is set as 2 μm in this paper.

## 3. Calculation of optical constants via Mie theory

Before starting the optical simulation of WLED, the optical constants of YAG@$SiO_2$ phosphor need to be calculated via Mie theory [19]. Following is the process of the optical constants calculation. YAG phosphor can emit yellow light while being excited by blue light, thereby, 460 nm and 550 nm incident light as the light resource are chosen in the calculation. Algorithm process of optical parameters calculation is shown in Fig. 2.

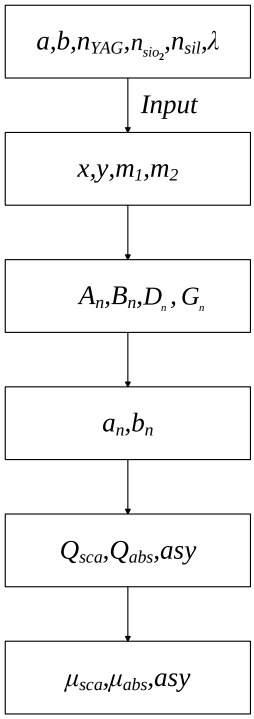


**Fig. 2 Algorithm process of optical parameters calculation**

Based on the size of YAG and YAG@$SiO_2$ phosphor ( $a$, $b$ ) , the refractive index of YAG($n_{YAG}$), $SiO_2$($n_{SiO_2}$) and silicone($n_{sil}$), the incident light wavelength in the ambient medium($\lambda$), the scattering efficiency( $Q_{sca}$ ), absorption efficiency( $Q_{abs}$ )and asymmetry parameters( $asy$ )of YAG or YAG@$SiO_2$ phosphor can be calculated via Mie theory. Furthermore, the absorption coefficient ($\mu_{abs}$), scattering coefficient($\mu_{sca}$) and asymmetry parameters ( $asy$ ) of YAG and YAG@$SiO_2$ phosphor can also be calculated by Mie theory. The specific calculation process is illustrated below.

According to Mie scattering theory, $x$, $y$ are the size constants, which can be calculated by equations ( 1 ) and ( 2 ) :

$$x = k \times a \tag{1}$$

$$y = k \times b \tag{2}$$

As shown in Fig. 1(c), $a$ is the radius of YAG phosphor and $b$ is the overall radius of YAG@$SiO_2$. In addition, $b$-$a$ is the coating thickness, $k$ is the wave number in the ambient medium (silicone gel) which can be described by equation (3):

$$k = \frac{2\pi n_{sil}}{\lambda} \tag{3}$$

where $\lambda$ is the incident light wavelength in the ambient medium. $n_{sil}$ is silicone gel's refractive index. $m_1$ is the refractive index of YAG phosphor relative to the ambient medium, $m_2$ is the refractive index of $SiO_2$ coating relative to the ambient medium. Silica gel is the ambient medium in LED packaging. Here the following equations (4) and (5) give the expression of $m_1$ and $m_2$.

$$m_1 = \frac{n_{YAG}}{n_{sil}} \tag{4}$$

$$m_2 = \frac{n_{SiO_2}}{n_{sil}} \tag{5}$$

YAG phosphor and $SiO_2$ both have scattering and absorption properties, so their refractive indices have a complex form:

$$n_{YAG} = n'_{YAG} - n''_{YAG} \times i \tag{6}$$

$$n_{SiO_2} = n'_{SiO_2} - n''_{SiO_2} \times i \tag{7}$$

where $n'$ and $n''$ are the refractive index and extinction coefficient. The relationship between $n'$ and $n''$ is shown as following:

$$n'' = \alpha\lambda / 4\pi n' \tag{8}$$

where $\alpha$ is absorption coefficient, $\lambda$ is the incident wavelength.

Table 1 lists the parameters of involved material. Most of the light can directly pass through the $SiO_2$ layer, the scattering effect is not obvious, and the scattering coefficient of $SiO_2$ is almost 0. As showed in Table 1, the transmittance($T$) of $SiO_2$ is close to 1 which means $SiO_2$ have good optical transparency. Meantime, $SiO_2$ almost has no absorption in the visible light range. The absorption coefficient ($\alpha$), refractive index($n'$) and extinction coefficient($n''$) were shown in table1 which can be used in calculation.

**Table 1** parameters of YAG and $SiO_2$[20-22]

| Components | parameters | |
|---|---|---|
| $SiO_2$ layer | $\lambda$ = 460 nm, $n'_{SiO_2}$ = 1.484, $n''_{SiO_2}$ = 4.00E-07 | $\alpha$ =0.162 cm$^{-1}$, $T$ =0.987 , |
| | $\lambda$ = 550 nm, $n'_{SiO_2}$ = 1.479, $n''_{SiO_2}$ = 4.00E-07 | $\alpha$ =0.1352 cm$^{-1}$, $T$ =0.991 |
| YAG | $\lambda$ = 460 nm, $n'_{YAG}$ = 1.851, $n''_{YAG}$ = 5.12E-04 | $\alpha$ =258.897 cm$^{-1}$ |
| | $\lambda$ = 550 nm, $n'_{YAG}$ = 1.839, $n''_{YAG}$ = 1.31E-05 | $\alpha$ =5.984 cm$^{-1}$ |

Here the following equations (9) to (12) give the expression for $A_n$, $B_n$, $D_n$ *and* $m$, where $\psi_n$ and $\chi_n$ are Bessel functions, $m$ is the refractive index with respect to the ambient medium, $D_n$ is the logarithmic derivative of $\psi_n$.

$$A_n = \psi_n(m_2x)\frac{mD_n(m_1x) - D_n(m_2x)}{mD_n(m_1x)\chi_n(m_2x) - \chi_n'(m_2x)} \tag{9}$$

$$B_n = \psi_n(m_2x)\frac{D_n(m_1x)/m - D_n(m_2x)}{D_n(m_1x)\chi_n(m_2x) - \chi_n'(m_2x)} \tag{10}$$

$$m = \frac{m_2}{m_1} \tag{11}$$

$$D_n = \frac{\psi'_n(mx)}{\psi_n(mx)} \tag{12}$$

Here the following equations (13) and (14) give the expression for $D_n$ and $G_n$.

$$\tilde{D}_n = \frac{D_n(m_2y) - \dfrac{A_n\chi_n'(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{A_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{13}$$

$$\tilde{G}_n = \frac{D_n(m_2y) - \dfrac{B_n\chi_n'(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{B_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{14}$$

In Mie scattering theory, $a_n$ and $b_n$ are the Mie expansion scattering coefficients. They could be expressed by equations (15) and (16):

$$a_n = \frac{(\tilde{D}_n / m_2 + n / y)\psi_n(y) - \psi_{n-1}(y)}{(\tilde{D}_n / m_2 + n / y)\xi_n(y) - \xi_{n-1}(y)} \tag{15}$$

$$b_n = \frac{(m_2 \tilde{G}_n + n / y)\psi_n(y) - \psi_{n-1}(y)}{(m_2 \tilde{G}_n + n / y)\xi_n(y) - \xi_{n-1}(y)} \tag{16}$$

where $\xi_n$ is Hankel functions of second kind.

According to Mie scattering theory, the extinction efficiency $Q_{ext}$, the scattering efficiency $Q_{sca}$, the absorption efficiency $Q_{abs}$, and the asymmetry parameter *asy* of optical medium are calculated according to equations (17) to (20) [22].

$$Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)\left(|a_n|^2 + |b_n|^2\right) \tag{17}$$

$$Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) Re\left(a_n + b_n\right) \tag{18}$$

$$Q_{abs} = Q_{ext} - Q_{sca} \tag{19}$$

$$asy = \frac{4}{x^2} \left\{ \sum_{n=1}^{\infty} Re(a_n a^*_{(n+1)} + b_n b^*_{(n+1)}) \right\} / Q_{sca} \tag{20}$$

Among them, $R_e$ represents the real part of the complex number, * represents the transpose.

Based on the results of $Q_{sca}$, and $Q_{abs}$, the absorption coefficient ($\mu_{abs}$) *and* scattering coefficient ($\mu_{sca}$) of YAG and YAG@$SiO_2$ are calculated according to equations (21) and (22)[22].

$$\mu_{abs} = Q_{abs} A v_f \cdot (1/V) = 3Q_{abs} v_f / 4b \tag{21}$$

$$\mu_{sca} = Q_{sca} A v_f \cdot (1/V) = 3Q_{sca} v_f / 4b \tag{22}$$

where *A* is the geometrical cross area of the phosphor particle, *V* is the volume of the particle , $v_f$ is the volume fraction of YAG or YAG@$SiO_2$. For YAG@$SiO_2$, $v_f$ is described by equation (23):

$$v_f = \frac{m_{YAG} / \rho_{YAG} + m_{SiO_2} / \rho_{SiO_2}}{m_{YAG} / \rho_{YAG} + m_{SiO_2} / \rho_{SiO_2} + m_{sil} / \rho_{sil}} \tag{23}$$

$m_{YAG}$ is the mass of YAG phosphor, $m_{SiO_2}$ is the mass of $SiO_2$, $m_{sil}$ is the mass of silica gel, $\rho_{YAG}$ is the density of YAG phosphor, $\rho_{SiO_2}$ is the density of $SiO_2$ and $\rho_{sil}$ is the density of silica gel. In this calculation, $\rho_{YAG}$ , $\rho_{SiO_2}$ and $\rho_{sil}$ are set as 4.6, 2.2 and 1.1 g/cm$^3$, respectively. In practical applications, mass fraction of YAG phosphor ($w_f$) in phosphor film is more commonly used instead of the volume fraction of phosphor ($v_f$), it is expressed as following:

$$w_f = \frac{m_{YAG} + m_{SiO_2}}{m_{YAG} + m_{SiO_2} + m_{Sil}} \tag{24}$$

The absorption coefficient ($\mu_{abs}$), scattering coefficient ($\mu_{sca}$) and asymmetry parameter ($asy$) of the phosphor film affect the light absorption and scattering, therefore, show great influence on the light extraction and the final luminous efficiency of WLED. Concentration of YAG phosphors and a, b values are the main factors that affect the optical constants $\mu_{abs}$ , $\mu_{sca}$ and $asy$ of the final fluorescent film. The influence of coating thickness (b-a), mass fraction of the phosphor ($w_f$) and incident light wavelength (λ) on $\mu_{abs}$ , $\mu_{sca}$ and $asy$ of phosphor film are discussed through Mie scattering theory calculation. Generally, 460nm blue light excites YAG phosphor and generates yellow light with a dominant wavelength of 550nm. For simplicity , 460 $\mu_{abs}$ and 550 $\mu_{abs}$ denote the absorption coefficient of phosphors excited by 460nm and 550nm incident light, respectively. 460 $\mu_{sca}$ and 550 $\mu_{sca}$ denote the scattering coefficient of phosphors excited by 460nm and 550nm incident light, respectively.

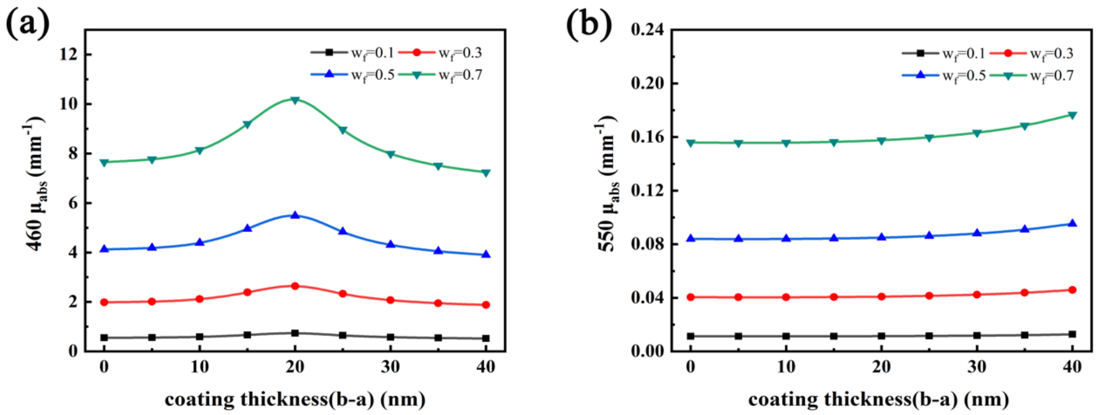


**Fig. 3** $\mu_{abs}$**of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig.3 (a), $460\mu_{abs}$ increased as the thickness of $SiO_2$ layer increased from 0 to 20 nm, and then decreased when continue increasing the thickness to 40 nm. It is obviously noticed that $460\mu_{abs}$ reached the highest value when the phosphor coating is 20nm. Compared with pristine phosphor , after being coated with nano-$SiO_2$ layer, the photons mainly transmit the $SiO_2$ layer via increasing the absorption of blue light due to the low refractive index of $SiO_2$ and then get to the phosphor surface , therefore, the effective excitation absorption of the phosphor via the $SiO_2$ layer occurred [9]. Based on Lambert-Beer's law, the transmitted light through a layer of coating is inversely proportional to the thickness of coating material. Although the coating layer can decrease the reflectance (which enhances the luminescence properties), while the quantity of light escaping from phosphor is reduced in much thicker layer [13]. Therefore, in our research, when the coating thickness is 20nm, the absorption of 460nm blue light by YAG@ $SiO_2$ find the maximum value. Our calculation is entirely consistent with previous reports [13,24].

The incident light absorption coefficient $460\mu_{abs}$ and $550\mu_{abs}$ are not in the same order of magnitude as shown in Fig.3. $550\mu_{abs}$ is much smaller than $460\mu_{abs}$. Meanwhile, as shown in Fig.3 (b), for 550nm incident light, the thickness of the $SiO_2$ coating layers had little influence on the absorption coefficient of YAG phosphor film. All these are due to the fact that YAG phosphor crystals show quite different absorption coefficients while excited by blue or yellow light [25, 26], for blue light the absorption coefficient is 3-8 $mm^{-1}$, however it is only 0.1-0.5 $mm^{-1}$ for yellow light. Our calculation is in accordance with the experimental results.

While considering about the influence of mass fraction of the phosphor ( $w_f$ ) on $460\mu_{abs}$ or $550\mu_{abs}$, as $w_f$ increased from 0.1 to 0.7, there are more phosphor particles in the fluorescent film, the absorption of incident light increased, thus, $460\mu_{abs}$ or $550\mu_{abs}$ increased accordingly.

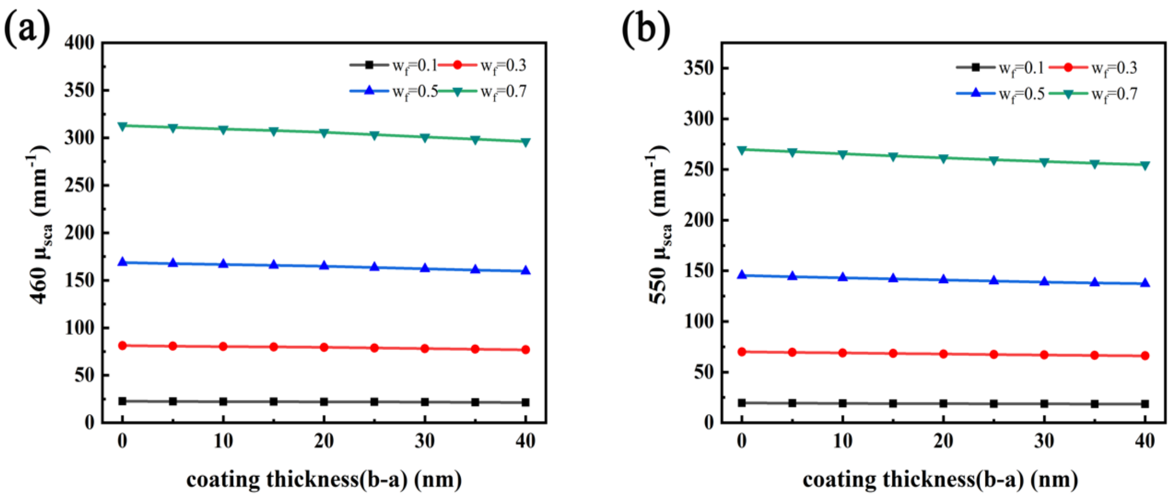


**Fig.4 $\mu_{sca}$ of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig. 4, when the thickness of the $SiO_2$ coating layer increased, $460\mu_{sca}$ and $550\mu_{sca}$ of YAG@$SiO_2$ both slightly decreased, illustrated that less light energy is lost by scattering and more energy can be used for illumination by coating thicker $SiO_2$ layer. It is noting that using phosphors with smaller scattering coefficient could be a way to suppress the scattering loss. The results indicated that coating of $SiO_2$ suppressed the scattering loss in a certain extent [22]. While increase $w_f$ of phosphor from 0.1 to 0.7, more light was scattered because there is more phosphor in the fluorescent film. Comparing the results in Fig.4 (a) and (b), it is found that the variation of $\mu_{sca}$ is very small when the incident light changes from blue light to yellow light. This indicates that the scattering property of coated phosphors are similar with uncoated one for different light, the big difference of absorption property between coated phosphor and uncoated one might be the main reason that affect the light extraction and luminous efficiency of WLED.

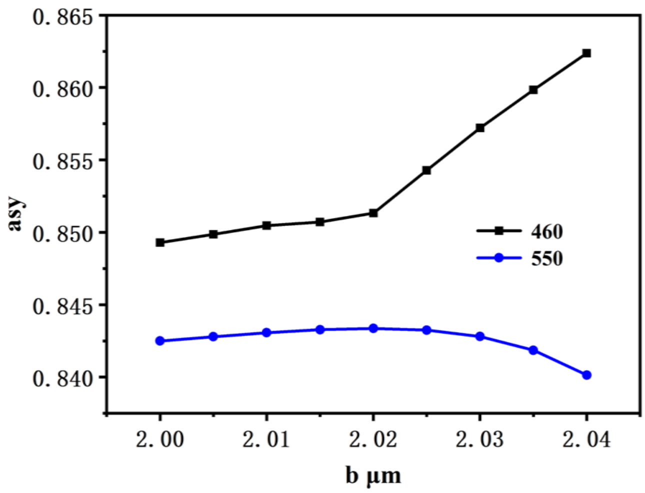


**Fig.5 Asymmetry parameter *asy* of phosphor film**

As shown in Fig.5, while excited by 460 nm or 550 nm incident light, *asy* of YAG and YAG@$SiO_2$ phosphor were positive, which meant under this condition, the number of forward scattered lights were greater than the number of backscattered lights [23]. While the coating thickness increased to 20nm, *asy* (460 nm or 550 nm excitation) increased a little, indicated the increasing of forward scattering. When coating thickness exceeded 20 nm, *asy* of YAG@$SiO_2$ had opposite trends while excited by 460 nm blue light or 550 nm yellow light. The increase of $asy_{460}$ indicated that the scattered light concentrated in smaller forward scattering angle, which resulted in an increase in the number of forward scattered light. Reversely, the decrease of $asy_{550}$ meant that more light was backscattered, absorbed and converted into heat loss. Herein, the backscattering loss of the emission from phosphor particles decreased the external quantum efficiency of the white LED [27]. If there are more forward scattered light existed in the packaged WLED, the luminous efficiency is improved as a result. The results in Fig.5 shows that the value of $asy_{550}$ and $asy_{460}$ is very close. When coating thickness changes, there is no great variation in *asy*. However, based on the previous results, it is clear that scattering property of phosphors is not the main reason for light extraction in packaged WLED. The tiny difference between $asy_{550}$ and $asy_{460}$ almost have no effect on light extraction in packaged WLED.

## 4. Optical simulation of CSP-packaged WLED

In most commercial optical software such as Light Tools and Trace Pro, the phosphor scattering is normally treated as Mie scattering to bring about the optical simulation of white LED packaging. The precise optical constants calculation via Mie theory could afford necessary supports for the optical simulation in LED packaging design.

Depend on these obtained optical constants $\mu_{abs}$, $\mu_{sca}$ and *asy*, we carried out the photoluminescence property simulation for YAG and YAG@$SiO_2$ WLED by Monte Carlo ray tracing method. The configuration of CSP-packaged WLED is given in Fig.6. The phosphor film is coated on the surface of the flip chip LED. The CSP chip is a 1 W blue LED chip or yellow LED chip (SAMSUNG LM101B) with dimension of 1mm×1mm×H mm, while H denotes the phosphor film thickness. The receiving surface (Receiver F) is assumed as a perfect absorber which collects blue light emitted from the blue LED chip and yellow light emitted from YAG or YAG@$SiO_2$ phosphor. To simplify the simulation, the radius of YAG particles is fixed at 2μm, coating thickness of YAG@$SiO_2$ is set at 20nm, mass fraction of the phosphor ($w_f$) in phosphor film is set at 0.7.

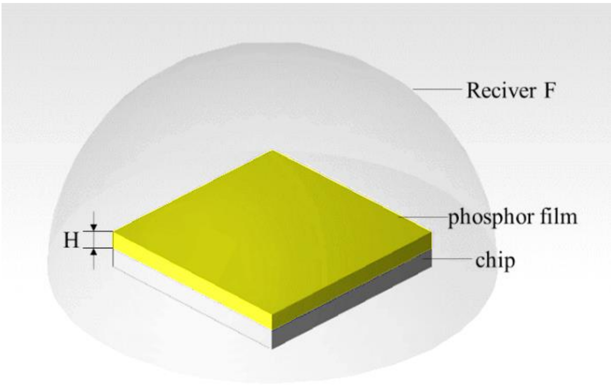


**Fig.6 C**onfiguration **of Chip-Scale-Packaged (CSP) WLED**

Generally, the most important thing in WLED packaging is the absorption and scattering properties of YAG phosphor for blue light emit from the chip and the yellow light emit from YAG phosphor itself. When the phosphor is excited by 460 nm blue light, the transmitted light is divided into two parts, unchanged blue light and converted yellow light. For 550 nm yellow light excitation, since no converted light is emitted from the phosphor film, the transmitted light is sorted as the yellow light. In this simulation, two 1W color LEDs with peak wavelength of 460 and 550nm are used as the light sources, coating thickness of YAG@$SiO_2$ is fixed at 20nm and the thickness of the phosphor film changes from 0.05 to 0.30 mm. The influence of the phosphor film thickness on light emission of CSP WLED was investigated and the results are shown in Fig.7. For the sake of simplicity, the transmittance for the unconverted blue light emit from blue LED and converted yellow light emit from phosphor are denoted as $\eta_{460\mathrm{BT}}$ and $\eta_{460YT}$. The transmittance of yellow light emit from yellow LED are denoted as $\eta_{550\mathrm{YT}}$. The total yellow light emits from phosphor excited by yellow LED are denoted as $\eta_{550\mathrm{Y}}$. The subscript of these signals, such as 460 and 550 indicate the excitation wavelength.

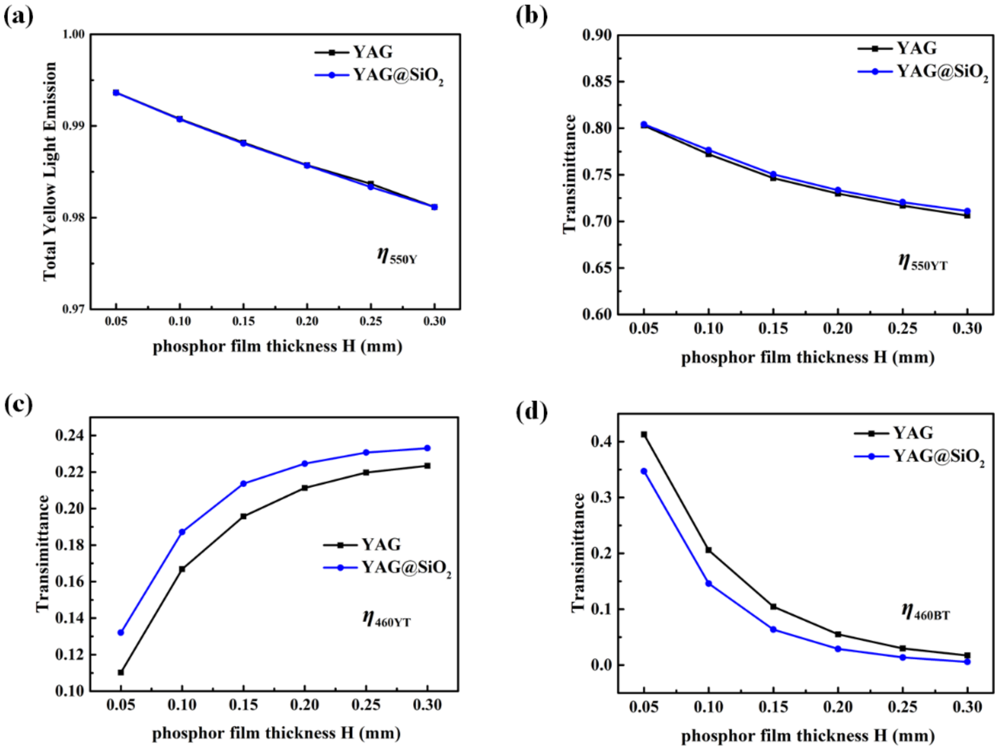


**Fig. 7** Simulation results of **(a)** Total yellow light emission from phosphor, the transmittance of YAG and YAG@$SiO_2$ phosphors for (b) yellow light emit from yellow LED (c) converted light emit from phosphor excited by blue light and (d) blue light emit from blue LED

As shown in Fig. 7 (a), when the phosphor is excited by 550nm yellow light, the total amount of yellow light scattered from YAG@$SiO_2$ phosphor is almost consistent with it from YAG phosphor. It is because $SiO_2$ almost has no absorption in the visible light range, hence, the absorption of yellow light by $SiO_2$ is negligible as shown in Fig. 7 (a). As seen from Table 1, the absorption coefficients of $SiO_2$ at 460nm and 550nm are basically the same, therefore, the absorption of 460nm blue light by the coated 20nm $SiO_2$ layer is also negligible.

As seen from the results of Fig.5, 550*asy* increase slightly while YAG phosphor was coated by 20nm $SiO_2$, indicates that under yellow light illumination, more of the light is forward scattered compared with pristine YAG phosphor. Therefore, as seen from Fig.7(b), $\eta_{550YT}$ of YAG@$SiO_2$ is slightly higher than that of YAG phosphor. Based on Lambert-Beer's law, more light is absorbed when the thickness of the phosphor film H increased from 0.05 to 0.3mm, therefore, $\eta_{550YT}$ of YAG and $YAG@SiO_2$ decreased as a result.

Fig. 7(c) and (d) show us the transmittance for the converted yellow light ($\eta_{460YT}$) and the unconverted blue light ($\eta_{460BT}$) excited by blue LED. It shows that $\eta_{460YT}$ increase but $\eta_{460BT}$ decrease while the phosphor film thickness increase. This is in accordance with the result of Lambert-Beer's law , while more blue light could be absorbed by phosphors as the phosphor film is thicker, therefore, less unconverted blue light but more converted yellow light emit out. When the phosphor film thickness is the same, $\eta_{460YT}$ of $YAG@SiO_2$ is greater than that of YAG. This is due to the fact that $YAG@SiO_2$ possess higher $460\mu_{abs}$ (see Fig.4(a)), hence more blue light is absorbed by $YAG@SiO_2$ compared with YAG, accordingly more light is converted into yellow light. The simulation results indicate that a thin $SiO_2$ layer does help to increase the yellow light emission, as many earlier scholars reported [13,24].

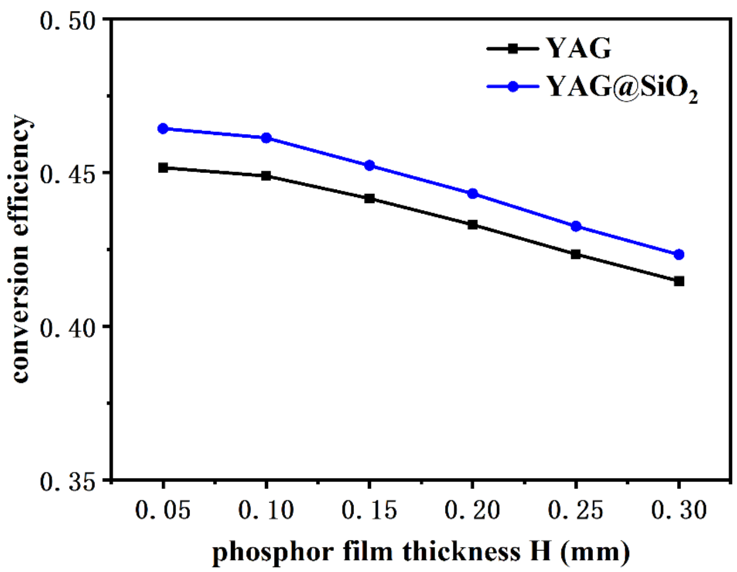


**Fig. 8 Conversion efficiency of phosphor**

Fig. 8 shows the conversion efficiency of YAG and $YAG@SiO_2$ excited by blue LED. As the thickness of the phosphor film increases, the conversion efficiency of phosphor gradually decreases, it might due to the fact that when the film is too thick or the phosphor concentration is too high, the oversaturated phosphor causes more converted light to be back reflected [21], and less light to be forward reflected. This might cause multiple reflection of the converted light between the phosphor layer and the chip. The multiple reflection result in the high absorption of converted light and decrease of luminous efficiency. However, YAG@$SiO_2$ has a 1.2% higher conversion efficiency than YAG, which implies that phosphor coating might be an effective way to improve the light efficiency.

In order to generate white light, the luminescence efficiency and true color map of the CSP WLED with different YAG film thickness ( H ) is simulated. As the thickness of the YAG fluorescent film increases, the luminous efficacy and color temperature of blue LED excited WLED gradually increase. When H is 0.3mm, the luminous efficiency gradually reaches saturation. When H is 0.2mm, the fabricated CSP LED possess a cold white light emission with a CCT of 10066K, color coordinates of (0.2851, 0.2786) ( as shown in Fig.11(b) ) and a luminous efficacy up to 130.3 lm/W (as shown in Fig.9).

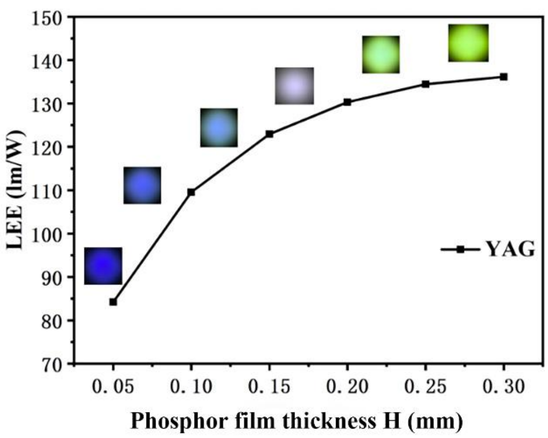


**Fig. 9 Influence of YAG fluorescent film thickness on luminous efficiency of YAG WLED**

The fluorescent film thickness (H) is fixed at 0.2mm, the influence of $SiO_2$ coating thickness on the luminous efficiency (LEE) and Correlate Color Temperature (CCT) of CSP WLED are shown in Fig.10. With the increasing of $SiO_2$ coating thickness, LEE of CSP WLED firstly increase and then decrease. When the coating thickness is 20nm, the luminous efficacy reached the maximum value 138.92 lm/W. This might due to the fact that $460\mu_{abs}$ of YAG@$SiO_2$ phosphor reaches the highest value while the $SiO_2$ coating thickness is 20 nm. Under this condition, more blue light emitted from the chip could be absorbed by YAG@$SiO_2$ phosphor film. More absorption of blue light by the YAG@$SiO_2$ phosphor, more emission of yellow light, therefore enhanced LEE is obtained.

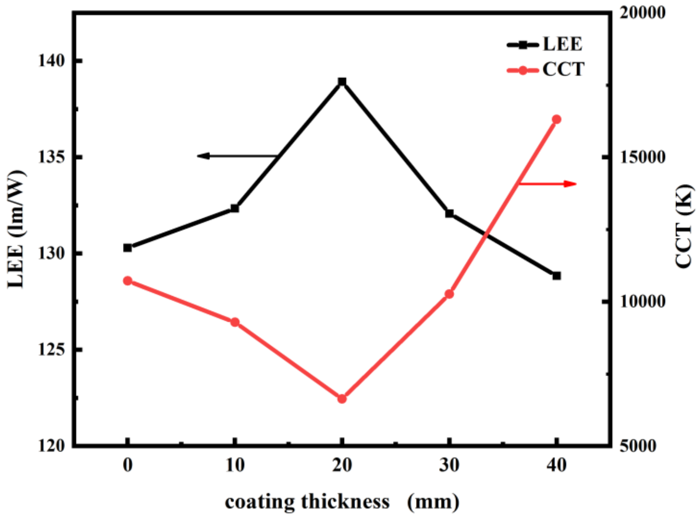


**Fig.10 Influence of coating thickness on LEE and CCT of CSP WLED**

Meanwhile, CCT of YAG@$SiO_2$ WLED decreases when the thickness of $SiO_2$ coating layer increases from 0 to 20 nm. When the thickness of the $SiO_2$ coating layer is over 20 nm, the color temperature of YAG@$SiO_2$ WLED increases sharply. Low color temperature WLED is prefer under working condition. It is found that proper $SiO_2$ layer thickness endowing YAG@$SiO_2$ with more absorption of blue light and high output of yellow light, therefore significantly enhance the LEE and decrease the

CCT of WLED. The highest value of LEE, 138.92 lm/W, the lowest CCT, 6667K, are achieved at a $SiO_2$ layer thickness of 20nm. The simulation results above show that proper $SiO_2$ coating on phosphors is responsible for the enhanced luminous efficacy and lower color temperature of CSP WLED, which is in accordance with the former reports. [23]

Using Monte Carlo method, the quality of white light emission from the YAG and YAG@$SiO_2$ WLED was evaluated via CIE chromaticity diagram and Luminous flux figure (as shown in Fig.11). The results are listed in Table 2.

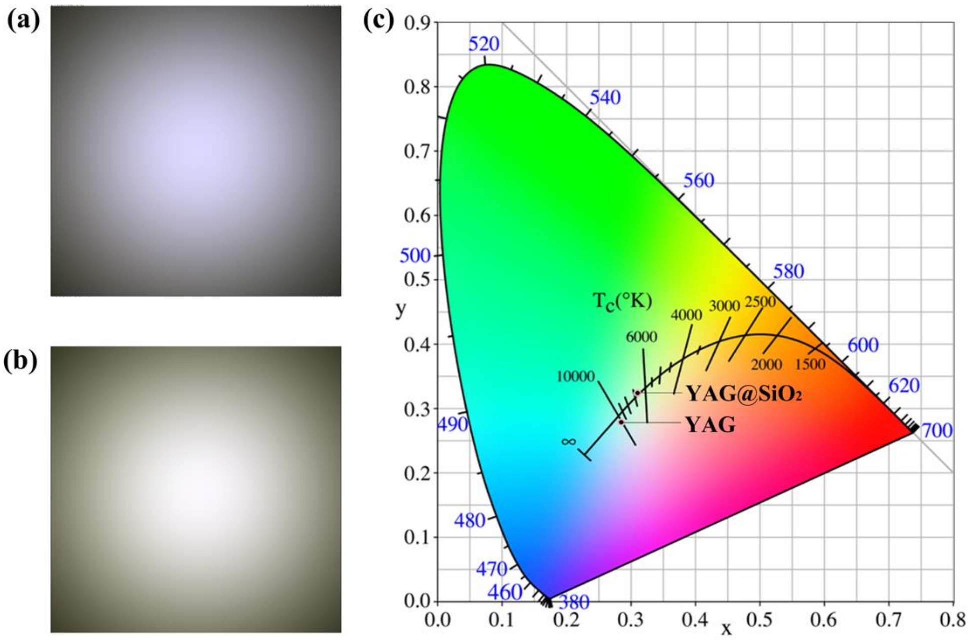


**Fig. 11 (a) Luminous flux figure of YAG WLED; (b)Luminous flux figure of YAG@$SiO_2$WLED; (c) Chromaticity color coordinates of YAG and YAG@$SiO_2$ upon excitation at 460 nm**

**Table. 2 Optical properties of YAG and YAG@$SiO_2$ WLEDs Simulated by Monta Carlo Ray Tracing method**

| Phosphor | LEE（lm/W） | CCT (K) | CIE (x, y) | Fluorescence conversion efficiency |
|---|---|---|---|---|
| YAG | 132.11 | 10066 | (0.2851,0.2786) | 0.4299 |
| YAG@$SiO_2$ | 138.92 | 6637 | (0.3110,0.3244) | 0.4392 |

When the thickness of fluorescent film is 0.2 mm, $SiO_2$ coating layer is 20 nm, YAG@$SiO_2$ WLED shows a light efficiency of 138.92 lm/W, a color temperature of 6637K, and a color coordinate of (0.3110, 0.3244), as shown in Tab.2. Compared with original YAG WLED, higher LEE and lower CCT is achieved in YAG@$SiO_2$ WLED, which is resulted from enhanced forward scattering and stronger blue light absorption. Meanwhile, the color coordinates of YAG@$SiO_2$ WLED is closer to the theoretical white point of (0.33, 0.33). This result shows that an ideal white color is almost achieved in YAG@$SiO_2$ under 460nm blue LED excitation. Meanwhile, proper $SiO_2$ thin layer coating on YAG significantly enhanced LEE and CCT of WLED, and a good cold white light emission is achieved.

Our simulation gives a theoretical explanation about the reason why proper coating thickness on YAG phosphor endows the CSP WLED with higher luminous efficacy and lower color temperature, hence better luminescence properties.

## 5. Conclusions

Optical configuration of chip scale packages WLEDs are established by coating YAG or YAG@$SiO_2$ phosphor film directly on the chip surface. In order to ensure the correct simulation of luminescence properties of the CSP white LED, the specific optical constants including the absorption coefficient $\mu_{abs}$, scattering coefficient $\mu_{sca}$, and anisotropy factor $asy$ of YAG and YAG@$SiO_2$ are calculated based on Mie scattering theory. The dependency of coating thickness of $SiO_2$ layer and phosphor mass fraction $w_f$ on optical constants $\mu_{abs}, \mu_{sca}$ and $asy$ are investigated. It shows that when the coating thickness is 20 nm, the absorption coefficient increases the most, which is conducive to increase the absorption of blue light, enhance the yellow light emission and eventually improve the luminescence property. The decrease in scattering coefficient is also conducive to the improvement of luminous efficiency. Numerical results show that Mie theory is effective in predicting the changing tendencies of the optical constants as the mass fraction of phosphor or the coating thickness changes. It makes Mie theory a suitable tool in WLED packaging design. Two color LEDs are used as light sources to simulate the light extraction of YAG and YAG@$SiO_2$ WLED via Monte Carlo ray tracing method. It implies that $SiO_2$ coating mainly result in the enhanced absorption of blue light and yellow light converting, hence the higher conversion efficiency for YAG@$SiO_2$. As the thickness of the fluorescent film is 0.2 mm, with 2 μm YAG@$SiO_2$ coated by 20 nm $SiO_2$ layer in it, our WLED gives a light efficiency of 138 lm/W, a color temperature of 6637 K, and a color coordinate of (0.3110, 0.3244), The light conversion efficiency after coating is increased by 1.2% compared with that before coating.

The simulation of photoluminescence property of YAG@$SiO_2$ WLED can be adapted to various coated phosphors WLED systems, the color quality can be easily tuned by changing the coating thickness, the phosphor film thickness or the mass fraction of phosphor, which have potential use in the future WLED packaging designing.

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# Simulation of Optical behavior of YAG:$Ce^{3+}$@$SiO_2$ phosphor used for chip scale packages WLED

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**Abstract**

YAG:$Ce^{3+}$ yellow phosphor are particularly used luminescent materials to produce white light in phosphor-converted white LED (pc-WLED). Surface coating of YAG phosphor is the main concern for desired optical performance of the phosphors. Many scholars conducted various experimental analysis on the surface coating of phosphors to improve yellow emission, but the theoretical explanation by which phosphor coating could help improving light efficiency has not yet been studied. In this paper, based on Mie theory, the optical constants such as scattering coefficient, absorption coefficient and asymmetry parameter of YAG:$Ce^{3+}$ phosphor and YAG@$SiO_2$ (YAG:$Ce^{3+}$ phosphor surface coated with nano-$SiO_2$ layer) were calculated. An optical configuration of chip scale packages (CSP) WLED was constructed by coupling YAG:$Ce^{3+}$ or YAG@$SiO_2$ phosphors with a LED laser. Based on the optical parameters calculated by Mie theory, the luminescent properties of YAG:$Ce^{3+}$ and YAG@$SiO_2$ WLED were simulated by Monte Carlo method. The results showed that a thin $SiO_2$ coating layer on YAG phosphor result in an overall increase in luminous performances compared with original YAG WLED. The absorption coefficient of phosphor is the main concern affecting the light

emission in WLED. Due to the fact that YAG@$SiO_2$ possess higher $460\mu_{abs}$, it could absorb more blue light than YAG, thereby it has a 1.2% higher conversion efficiency than YAG, finally the enhanced luminous efficiency of YAG@$SiO_2$ WLED is obtained. The results obtained in this work provides a potential method in future WLED packaging designing.

## 1. Introduction

White lighting-emitting-diode (WLED) has been widely used in commercial solid lighting applications because of its small size, long life, energy saving, environmentally friendly and high luminous efficiency properties [1, 2]. The most appropriate method to obtain WLED is called phosphor-converted (pc-) WLED. Typically, a pc-WLED is usually fabricated by combining the blue LED chip with YAG:$Ce^{3+}$ phosphors which has acceptable color rendering and robust reliability. Traditionally, a pc-WLED package consists of LED chip, phosphors, lead frame, silicone, substrate and so on [3]. However, more packaging components in WLED package indicate higher failure possibility as well as more space occupation and more weight[4]. The chip scale package (CSP) technology is developed by covering a thin YAG fluorescent film on a blue LED chip, which could tackle this problem. The advantages of CSP WLED are the increased manufacturing efficiency [5, 6], high packing density and high luminous flux output. In the package, refractive index of silica gel (1.41) is lower than that of YAG:$Ce^{3+}$ crystal (1.84) in the thin phosphor film, therefore, more yellow light is absorbed by phosphor particle due to the total internal reflection (TIR), luminous efficiency of the CSP WLED decreases accordingly. At the same time, the refractive index difference between phosphor and silica gel leads to light scattering at the interface, which also results in the blue light reflection loss and the decrease of luminous efficiency [7]. More recently, some studies try to solve the problem by coating a dielectric layer with suitable refractive index on the phosphor. This refers to coating one or more layers of oxide material on the surface of the phosphor particles, such as $TiO_2$ [8, 9], $Al_2O_3$ [10, 11] and $SiO_2$ [12, 13]. The oxide material coating on the phosphors with matched refractive index could reduce the yellow light absorption by TIR, decrease the blue light reflection loss at the interface, in the end, improve the luminous efficiency of WLED. Among them, $SiO_2$ is widely used due to its optical transparency, tunable size [14] and low cost [15]. It has been have concluded that $SiO_2$-coated YAG phosphor limits the thermal quenching properties[16, 17]. Therefore, YAG phosphor coated with $SiO_2$ layer(YAG@$SiO_2$) could be considered as a good candidate for white light-emitting diode applications[18]. Many scholars conducted experimental analysis on phosphor coating, most of the studies focus on the influence of oxide layer microstructure on the luminous efficiency of WLED evaluated by photoluminescence spectra (PL spectra), but no one go deep into the light efficiency enhancement mechanism investigations. Few researchers seriously considered how the variation of light absorption and scattering of oxide layer coated phosphor affect the light extraction of WLED. Meanwhile, the optical parameters such as scattering coefficient ($\mu_{sca}$), absorption coefficient ($\mu_{abs}$) and anisotropy parameter ($\mu_{abs}$)of the coated phosphors also change as well. Actually, precise optical constants of coated phosphor are indispensable in the numerical simulation of the luminescent property of WLED. However, few research discussed about this, to the best of our knowledge.

In this paper, the YAG:$Ce^{3+}$ and YAG@$SiO_2$ were chosen as the optical simulation target. Firstly, consider the YAG and YAG@$SiO_2$ phosphor as spheres, the optical constants of these two phosphors were calculated based on Mie theory. Secondly, based on the optical constants of YAG and YAG@$SiO_2$ phosphor obtained, the luminescence performances of YAG and YAG@$SiO_2$ CSP WLED were simulated based on Monte Carlo method. Thirdly, in view of the foregoing results, we hold the opinion that this method can be extended to other coating layers and phosphor systems and it is helpful to decrease the amount of experiments significantly.

## 2. Description of the configuration of CSP-packaged WLED

The configuration of CSP-packaged WLED is constructed as shown in Fig. 1. In CSP LEDs, blue LED chips are mostly covered with yellow YAG fluorescent film to generate white emission (as shown in Fig.1 (e)). The YAG fluorescent film (as shown in Fig. 1(d)) is composed of phosphor particles and silica gel which are mixed in certain proportion. The optical parameters of YAG phosphor film determines the light-emitting behavior (luminous efficiency, color temperature, etc.) of the final CSP WLED. After YAG phosphor is coated by $SiO_2$ layer (as shown in Fig.1(b), the optical constants of YAG@$SiO_2$ change accordingly, which can be calculated via Mie theory.

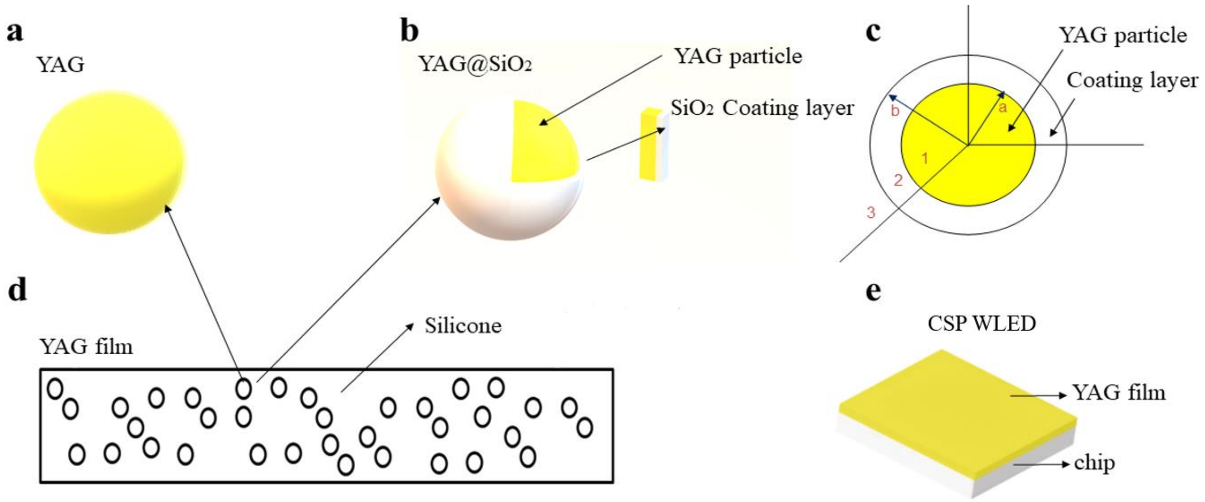


**Fig. 1 Schematic diagram of (a) YAG phosphor particle (YAG); (b) YAG phosphor coated with $SiO_2$ (YAG@$SiO_2$); (c) YAG@$SiO_2$ cross sectional view; (d) YAG film (e) CSP WLED**

We assume that spherical YAG and YAG@$SiO_2$ (YAG phosphor coated with a 10~40 nm $SiO_2$ layer) phosphor are evenly distributed in this film (as showed in Fig.1 (a) and (b)), where the yellow region is YAG phosphor and the white one is $SiO_2$ layer (as shown in Fig.1(b)). The sectional view of YAG@$SiO_2$ is shown in Fig. 1(c), in which signal 1,2,3 represent the fluorescent material (YAG), coating layer material ($SiO_2$) and silicone respectively, a and b represent the radius of YAG and YAG@$SiO_2$ phosphor, respectively.

To be convenient, we assume that, first of all, the nano-$SiO_2$ layer coated on the surface of YAG phosphor is optically transparent in the visible light range. Secondly, YAG and YAG@$SiO_2$ phosphor are ideal smooth spheres, meanwhile, $SiO_2$ layer are tightly contacted with YAG phosphor in YAG@$SiO_2$. The schematic diagram of phosphor film is shown in Fig. 1 (d). The phosphor film is consisted of phosphor particles and silicone, while the YAG phosphor particle size is set as 2 μm in this paper.

## 3. Calculation of optical constants via Mie theory

Before starting the optical simulation of WLED, the optical constants of YAG@$SiO_2$ phosphor need to be calculated via Mie theory [19]. Following is the process of the optical constants calculation. YAG phosphor can emit yellow light while being excited by blue light, thereby, 460 nm and 550 nm incident light as the light resource are chosen in the calculation. Algorithm process of optical parameters calculation is shown in Fig. 2.

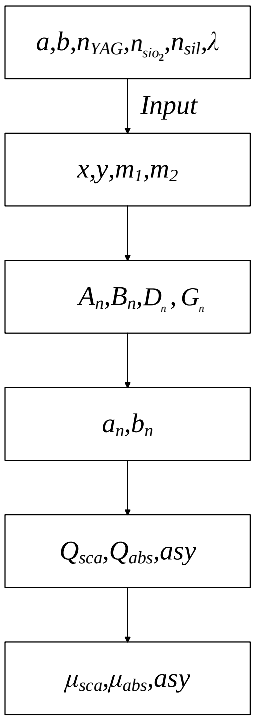


**Fig. 2 Algorithm process of optical parameters calculation**

Based on the size of YAG and YAG@$SiO_2$ phosphor（$a$, $b$）, the refractive index of YAG($n_{YAG}$), $SiO_2$($n_{SiO_2}$) and silicone($n_{sil}$), the incident light wavelength in the ambient medium($\lambda$), the scattering efficiency（$Q_{sca}$）, absorption efficiency（$Q_{abs}$）and asymmetry parameters（$asy$）of YAG or YAG@$SiO_2$ phosphor can be calculated via Mie theory. Furthermore, the absorption coefficient ($\mu_{abs}$), scattering coefficient($\mu_{sca}$) and asymmetry parameters（$asy$）of YAG and YAG@$SiO_2$ phosphor can also be calculated by Mie theory. The specific calculation process is illustrated below.

According to Mie scattering theory, $x$, $y$ are the size constants, which can be calculated by equations（1）and（2）:

$$x = k \times a \tag{1}$$

$$y = k \times b \tag{2}$$

As shown in Fig. 1(c), $a$ is the radius of YAG phosphor and $b$ is the overall radius of YAG@$SiO_2$. In addition, $b$-$a$ is the coating thickness, $k$ is the wave number in the ambient medium (silicone gel) which can be described by equation (3):

$$k = \frac{2\pi n_{sil}}{\lambda} \tag{3}$$

where $\lambda$ is the incident light wavelength in the ambient medium. $n_{sil}$ is silicone gel's refractive index. $m_1$ is the refractive index of YAG phosphor relative to the ambient medium, $m_2$ is the refractive index of $SiO_2$ coating relative to the ambient medium. Silica gel is the ambient medium in LED packaging. Here the following equations (4) and (5) give the expression of $m_1$ and $m_2$.

$$m_1 = \frac{n_{YAG}}{n_{sil}} \tag{4}$$

$$m_2 = \frac{n_{SiO_2}}{n_{sil}} \tag{5}$$

YAG phosphor and $SiO_2$ both have scattering and absorption properties, so their refractive indices have a complex form:

$$n_{YAG} = n'_{YAG} - n''_{YAG} \times i \tag{6}$$

$$n_{SiO_2} = n'_{SiO_2} - n''_{SiO_2} \times i \tag{7}$$

where $n'$ and $n''$ are the refractive index and extinction coefficient. The relationship between $n'$ and $n''$ is shown as following:

$$n'' = \alpha\lambda / 4\pi n' \tag{8}$$

where $\alpha$ is absorption coefficient, $\lambda$ is the incident wavelength.

Table 1 lists the parameters of involved material. Most of the light can directly pass through the $SiO_2$ layer, the scattering effect is not obvious, and the scattering coefficient of $SiO_2$ is almost 0. As showed in Table 1, the transmittance($T$) of $SiO_2$ is close to 1 which means $SiO_2$ have good optical transparency. Meantime, $SiO_2$ almost has no absorption in the visible light range. The absorption coefficient ($\alpha$), refractive index($n'$) and extinction coefficient($n''$) were shown in table1 which can be used in calculation.

**Table 1** parameters of YAG and $SiO_2$[20-22]

| Components | parameters | |
|---|---|---|
| $SiO_2$ layer | $\lambda$ = 460 nm, $n'_{SiO_2}$ = 1.484, $n''_{SiO_2}$ = 4.00E-07 | $\alpha$ =0.162 cm$^{-1}$, $T$ =0.987 , |
| | $\lambda$ = 550 nm, $n'_{SiO_2}$ = 1.479, $n''_{SiO_2}$ = 4.00E-07 | $\alpha$ =0.1352 cm$^{-1}$, $T$ =0.991 |
| YAG | $\lambda$ = 460 nm, $n'_{YAG}$ = 1.851, $n''_{YAG}$ = 5.12E-04 | $\alpha$ =258.897 cm$^{-1}$ |
| | $\lambda$ = 550 nm, $n'_{YAG}$ = 1.839, $n''_{YAG}$ = 1.31E-05 | $\alpha$ =5.984 cm$^{-1}$ |

Here the following equations (9) to (12) give the expression for $A_n$, $B_n$, $D_n$ *and* $m$, where $\psi_n$ and $\chi_n$ are Bessel functions, $m$ is the refractive index with respect to the ambient medium, $D_n$ is the logarithmic derivative of $\psi_n$.

$$A_n = \psi_n(m_2x)\frac{mD_n(m_1x) - D_n(m_2x)}{mD_n(m_1x)\chi_n(m_2x) - \chi_n'(m_2x)} \tag{9}$$

$$B_n = \psi_n(m_2x)\frac{D_n(m_1x)/m - D_n(m_2x)}{D_n(m_1x)\chi_n(m_2x) - \chi_n'(m_2x)} \tag{10}$$

$$m = \frac{m_2}{m_1} \tag{11}$$

$$D_n = \frac{\psi'_n(mx)}{\psi_n(mx)} \tag{12}$$

Here the following equations (13) and (14) give the expression for $D_n$ and $G_n$.

$$\tilde{D}_n = \frac{D_n(m_2y) - \dfrac{A_n\chi_n'(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{A_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{13}$$

$$\tilde{G}_n = \frac{D_n(m_2y) - \dfrac{B_n\chi_n'(m_2y)}{\psi_n(m_2y)}}{1 - \dfrac{B_n\chi_n(m_2y)}{\psi_n(m_2y)}} \tag{14}$$

In Mie scattering theory, $a_n$ and $b_n$ are the Mie expansion scattering coefficients. They could be expressed by equations (15) and (16):

$$a_n = \frac{(\tilde{D}_n / m_2 + n/y)\psi_n(y) - \psi_{n-1}(y)}{(\tilde{D}_n / m_2 + n/y)\xi_n(y) - \xi_{n-1}(y)} \tag{15}$$

$$b_n = \frac{(m_2 \tilde{G}_n + n/y)\psi_n(y) - \psi_{n-1}(y)}{(m_2 \tilde{G}_n + n/y)\xi_n(y) - \xi_{n-1}(y)} \tag{16}$$

where $\xi_n$ is Hankel functions of second kind.

According to Mie scattering theory, the extinction efficiency $Q_{ext}$, the scattering efficiency $Q_{sca}$, the absorption efficiency $Q_{abs}$, and the asymmetry parameter *asy* of optical medium are calculated according to equations (17) to (20) [22].

$$Q_{sca} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)\left(|a_n|^2 + |b_n|^2\right) \tag{17}$$

$$Q_{ext} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)Re\left(a_n + b_n\right) \tag{18}$$

$$Q_{abs} = Q_{ext} - Q_{sca} \tag{19}$$

$$asy = \frac{4}{x^2}\left\{\sum_{n=1}^{\infty} Re(a_n a^*_{(n+1)} + b_n b^*_{(n+1)})\right\} / Q_{sca} \tag{20}$$

Among them, $R_e$ represents the real part of the complex number, * represents the transpose.

Based on the results of $Q_{sca}$, and $Q_{abs}$, the absorption coefficient ($\mu_{abs}$) *and* scattering coefficient ($\mu_{sca}$) of YAG and YAG@$SiO_2$ are calculated according to equations (21) and (22)[22].

$$\mu_{abs} = Q_{abs} A v_f \cdot (1/V) = 3Q_{abs} v_f / 4b \tag{21}$$

$$\mu_{sca} = Q_{sca} A v_f \cdot (1/V) = 3Q_{sca} v_f / 4b \tag{22}$$

where $A$ is the geometrical cross area of the phosphor particle, $V$ is the volume of the particle , $v_f$ is the volume fraction of YAG or YAG@$SiO_2$. For YAG@$SiO_2$, $v_f$ is described by equation (23):

$$v_f = \frac{m_{YAG} / \rho_{YAG} + m_{SiO_2} / \rho_{SiO_2}}{m_{YAG} / \rho_{YAG} + m_{SiO_2} / \rho_{SiO_2} + m_{sil} / \rho_{sil}} \tag{23}$$

$m_{YAG}$ is the mass of YAG phosphor, $m_{SiO_2}$ is the mass of $SiO_2$, $m_{sil}$ is the mass of silica gel, $\rho_{YAG}$ is the density of YAG phosphor, $\rho_{SiO_2}$ is the density of $SiO_2$ and $\rho_{sil}$ is the density of silica gel. In this calculation, $\rho_{YAG}$ , $\rho_{SiO_2}$ and $\rho_{sil}$ are set as 4.6, 2.2 and 1.1 g/cm$^3$, respectively. In practical applications, mass fraction of YAG phosphor ($w_f$) in phosphor film is more commonly used instead of the volume fraction of phosphor ($v_f$), it is expressed as following:

$$w_f = \frac{m_{YAG} + m_{SiO_2}}{m_{YAG} + m_{SiO_2} + m_{Sil}} \tag{24}$$

The absorption coefficient ($\mu_{abs}$), scattering coefficient ($\mu_{sca}$) and asymmetry parameter ($asy$) of the phosphor film affect the light absorption and scattering, therefore, show great influence on the light extraction and the final luminous efficiency of WLED. Concentration of YAG phosphors and a, b values are the main factors that affect the optical constants $\mu_{abs}$ , $\mu_{sca}$ and *asy* of the final fluorescent film. The influence of coating thickness (b-a), mass fraction of the phosphor ($w_f$) and incident light wavelength (λ) on $\mu_{abs}$ , $\mu_{sca}$ and *asy* of phosphor film are discussed through Mie scattering theory calculation. Generally, 460nm blue light excites YAG phosphor and generates yellow light with a dominant wavelength of 550nm. For simplicity , 460 $\mu_{abs}$ and 550 $\mu_{abs}$ denote the absorption coefficient of phosphors excited by 460nm and 550nm incident light, respectively. 460 $\mu_{sca}$ and 550 $\mu_{sca}$ denote the scattering coefficient of phosphors excited by 460nm and 550nm incident light, respectively.

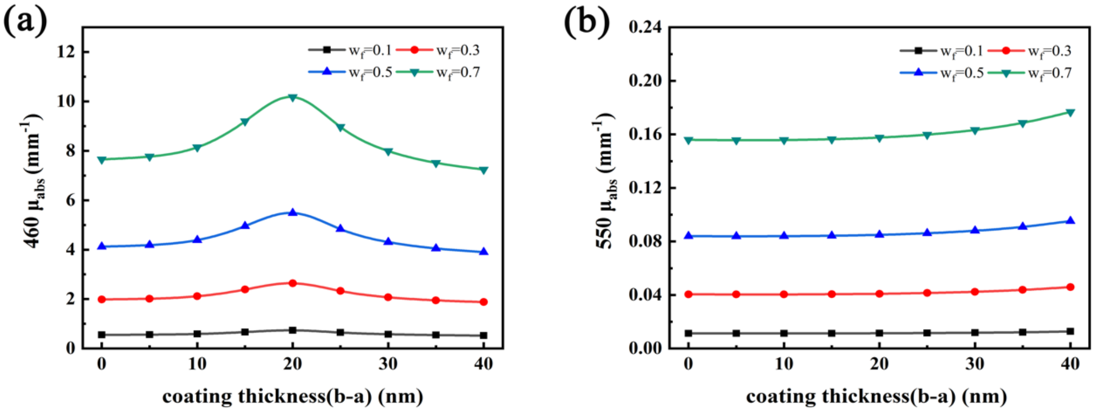


**Fig. 3** $\mu_{abs}$ **of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig.3 (a), $460\mu_{abs}$ increased as the thickness of $SiO_2$ layer increased from 0 to 20 nm, and then decreased when continue increasing the thickness to 40 nm. It is obviously noticed that $460\mu_{abs}$ reached the highest value when the phosphor coating is 20nm. Compared with pristine phosphor , after being coated with nano-$SiO_2$ layer, the photons mainly transmit the $SiO_2$ layer via increasing the absorption of blue light due to the low refractive index of $SiO_2$ and then get to the phosphor surface , therefore, the effective excitation absorption of the phosphor via the $SiO_2$ layer occurred [9]. Based on Lambert-Beer's law, the transmitted light through a layer of coating is inversely proportional to the thickness of coating material. Although the coating layer can decrease the reflectance (which enhances the luminescence properties), while the quantity of light escaping from phosphor is reduced in much thicker layer [13]. Therefore, in our research, when the coating thickness is 20nm, the absorption of 460nm blue light by YAG@ $SiO_2$ find the maximum value. Our calculation is entirely consistent with previous reports [13,24].

The incident light absorption coefficient $460\mu_{abs}$ and $550\mu_{abs}$ are not in the same order of magnitude as shown in Fig.3. $550\mu_{abs}$ is much smaller than $460\mu_{abs}$. Meanwhile, as shown in Fig.3 (b), for 550nm incident light, the thickness of the $SiO_2$ coating layers had little influence on the absorption coefficient of YAG phosphor film. All these are due to the fact that YAG phosphor crystals show quite different absorption coefficients while excited by blue or yellow light [25, 26], for blue light the absorption coefficient is 3-8 $mm^{-1}$, however it is only 0.1-0.5 $mm^{-1}$ for yellow light. Our calculation is in accordance with the experimental results.

While considering about the influence of mass fraction of the phosphor ( $w_f$ ) on $460\mu_{abs}$ or $550\mu_{abs}$, as $w_f$ increased from 0.1 to 0.7, there are more phosphor particles in the fluorescent film, the absorption of incident light increased, thus, $460\mu_{abs}$ or $550\mu_{abs}$ increased accordingly.

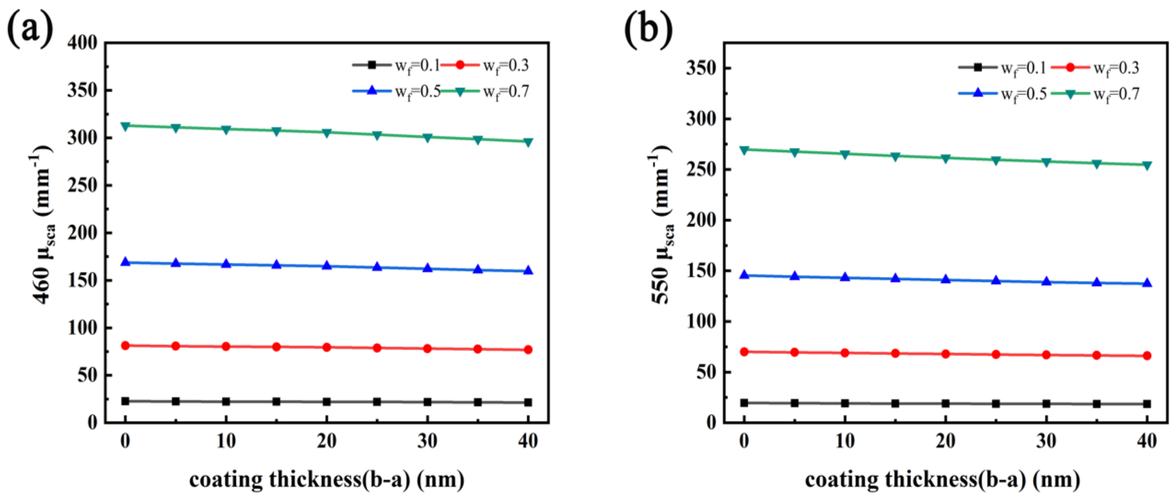


**Fig.4** $\mu_{sca}$ **of phosphor film (a) excited by 460nm blue light (b) excited by 550nm yellow light**

As shown in Fig. 4, when the thickness of the $SiO_2$ coating layer increased, $460\mu_{sca}$ and $550\mu_{sca}$ of YAG@$SiO_2$ both slightly decreased, illustrated that less light energy is lost by scattering and more energy can be used for illumination by coating thicker $SiO_2$ layer. It is noting that using phosphors with smaller scattering coefficient could be a way to suppress the scattering loss. The results indicated that coating of $SiO_2$ suppressed the scattering loss in a certain extent [22]. While increase $w_f$ of phosphor from 0.1 to 0.7, more light was scattered because there is more phosphor in the fluorescent film. Comparing the results in Fig.4 (a) and (b), it is found that the variation of $\mu_{sca}$ is very small when the incident light changes from blue light to yellow light. This indicates that the scattering property of coated phosphors are similar with uncoated one for different light, the big difference of absorption property between coated phosphor and uncoated one might be the main reason that affect the light extraction and luminous efficiency of WLED.

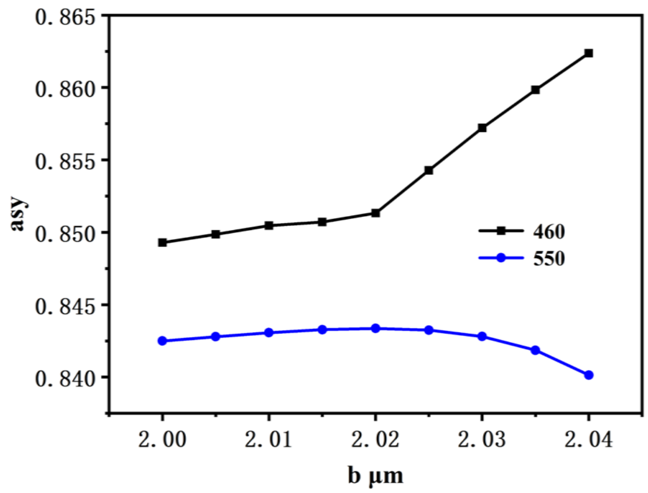


**Fig.5 Asymmetry parameter *asy* of phosphor film**

As shown in Fig.5, while excited by 460 nm or 550 nm incident light, *asy* of YAG and YAG@$SiO_2$ phosphor were positive, which meant under this condition, the number of forward scattered lights were greater than the number of backscattered lights [23]. While the coating thickness increased to 20nm, *asy* (460 nm or 550 nm excitation) increased a little, indicated the increasing of forward scattering. When coating thickness exceeded 20 nm, *asy* of YAG@$SiO_2$ had opposite trends while excited by 460 nm blue light or 550 nm yellow light. The increase of $asy_{460}$ indicated that the scattered light concentrated in smaller forward scattering angle, which resulted in an increase in the number of forward scattered light. Reversely, the decrease of $asy_{550}$ meant that more light was backscattered, absorbed and converted into heat loss. Herein, the backscattering loss of the emission from phosphor particles decreased the external quantum efficiency of the white LED [27]. If there are more forward scattered light existed in the packaged WLED, the luminous efficiency is improved as a result. The results in Fig.5 shows that the value of $asy_{550}$ and $asy_{460}$ is very close. When coating thickness changes, there is no great variation in *asy*. However, based on the previous results, it is clear that scattering property of phosphors is not the main reason for light extraction in packaged WLED. The tiny difference between $asy_{550}$ and $asy_{460}$ almost have no effect on light extraction in packaged WLED.

## 4. Optical simulation of CSP-packaged WLED

In most commercial optical software such as Light Tools and Trace Pro, the phosphor scattering is normally treated as Mie scattering to bring about the optical simulation of white LED packaging. The precise optical constants calculation via Mie theory could afford necessary supports for the optical simulation in LED packaging design.

Depend on these obtained optical constants $\mu_{abs}$ , $\mu_{sca}$ and *asy*, we carried out the photoluminescence property simulation for YAG and YAG@$SiO_2$ WLED by Monte Carlo ray tracing method. The configuration of CSP-packaged WLED is given in Fig.6. The phosphor film is coated on the surface of the flip chip LED. The CSP chip is a 1 W blue LED chip or yellow LED chip (SAMSUNG LM101B) with dimension of 1mm×1mm×H mm, while H denotes the phosphor film thickness. The receiving surface (Receiver F) is assumed as a perfect absorber which collects blue light emitted from the blue LED chip and yellow light emitted from YAG or YAG@$SiO_2$ phosphor. To simplify the simulation, the radius of YAG particles is fixed at 2μm, coating thickness of YAG@$SiO_2$ is set at 20nm, mass fraction of the phosphor ($w_f$) in phosphor film is set at 0.7.

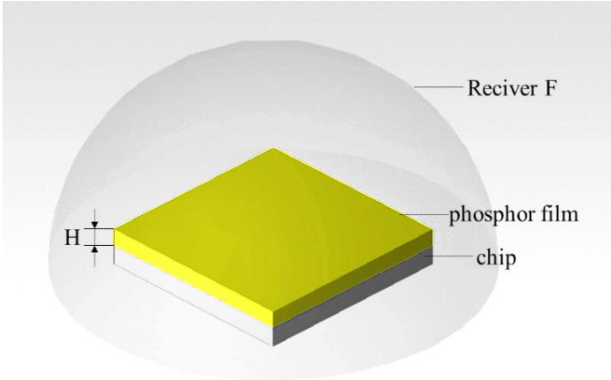


**Fig.6 C**onfiguration **of Chip-Scale-Packaged (CSP) WLED**

Generally, the most important thing in WLED packaging is the absorption and scattering properties of YAG phosphor for blue light emit from the chip and the yellow light emit from YAG phosphor itself. When the phosphor is excited by 460 nm blue light, the transmitted light is divided into two parts, unchanged blue light and converted yellow light. For 550 nm yellow light excitation, since no converted light is emitted from the phosphor film, the transmitted light is sorted as the yellow light. In this simulation, two 1W color LEDs with peak wavelength of 460 and 550nm are used as the light sources, coating thickness of YAG@$SiO_2$ is fixed at 20nm and the thickness of the phosphor film changes from 0.05 to 0.30 mm. The influence of the phosphor film thickness on light emission of CSP WLED was investigated and the results are shown in Fig.7. For the sake of simplicity, the transmittance for the unconverted blue light emit from blue LED and converted yellow light emit from phosphor are denoted as $\eta_{460\mathrm{BT}}$ and $\eta_{460YT}$. The transmittance of yellow light emit from yellow LED are denoted as $\eta_{550\mathrm{YT}}$. The total yellow light emits from phosphor excited by yellow LED are denoted as $\eta_{550\mathrm{Y}}$. The subscript of these signals, such as 460 and 550 indicate the excitation wavelength.

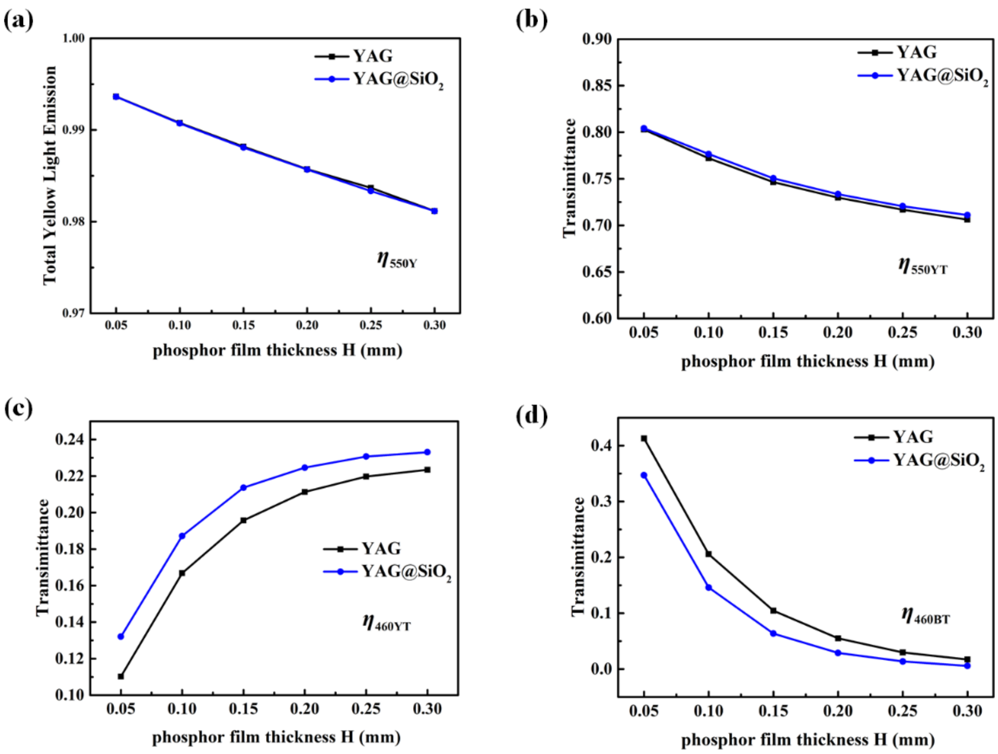


**Fig. 7** Simulation results of **(a)** Total yellow light emission from phosphor, the transmittance of YAG and YAG@$SiO_2$ phosphors for (b) yellow light emit from yellow LED (c) converted light emit from phosphor excited by blue light and (d) blue light emit from blue LED

As shown in Fig. 7 (a), when the phosphor is excited by 550nm yellow light, the total amount of yellow light scattered from YAG@$SiO_2$ phosphor is almost consistent with it from YAG phosphor. It is because $SiO_2$ almost has no absorption in the visible light range, hence, the absorption of yellow light by $SiO_2$ is negligible as shown in Fig. 7 (a). As seen from Table 1, the absorption coefficients of $SiO_2$ at 460nm and 550nm are basically the same, therefore, the absorption of 460nm blue light by the coated 20nm $SiO_2$ layer is also negligible.

As seen from the results of Fig.5, 550*asy* increase slightly while YAG phosphor was coated by 20nm $SiO_2$, indicates that under yellow light illumination, more of the light is forward scattered compared with pristine YAG phosphor. Therefore, as seen from Fig.7(b), $\eta_{550YT}$ of YAG@$SiO_2$ is slightly higher than that of YAG phosphor. Based on Lambert-Beer's law, more light is absorbed when the thickness of the phosphor film H increased from 0.05 to 0.3mm, therefore, $\eta_{550YT}$ of YAG and $YAG@SiO_2$ decreased as a result.

Fig. 7(c) and (d) show us the transmittance for the converted yellow light ($\eta_{460YT}$) and the unconverted blue light ($\eta_{460BT}$) excited by blue LED. It shows that $\eta_{460YT}$ increase but $\eta_{460BT}$ decrease while the phosphor film thickness increase. This is in accordance with the result of Lambert-Beer's law , while more blue light could be absorbed by phosphors as the phosphor film is thicker, therefore, less unconverted blue light but more converted yellow light emit out. When the phosphor film thickness is the same, $\eta_{460YT}$ of $YAG@SiO_2$ is greater than that of YAG. This is due to the fact that $YAG@SiO_2$ possess higher $460\mu_{abs}$ (see Fig.4(a)), hence more blue light is absorbed by $YAG@SiO_2$ compared with YAG, accordingly more light is converted into yellow light. The simulation results indicate that a thin $SiO_2$ layer does help to increase the yellow light emission, as many earlier scholars reported [13,24].

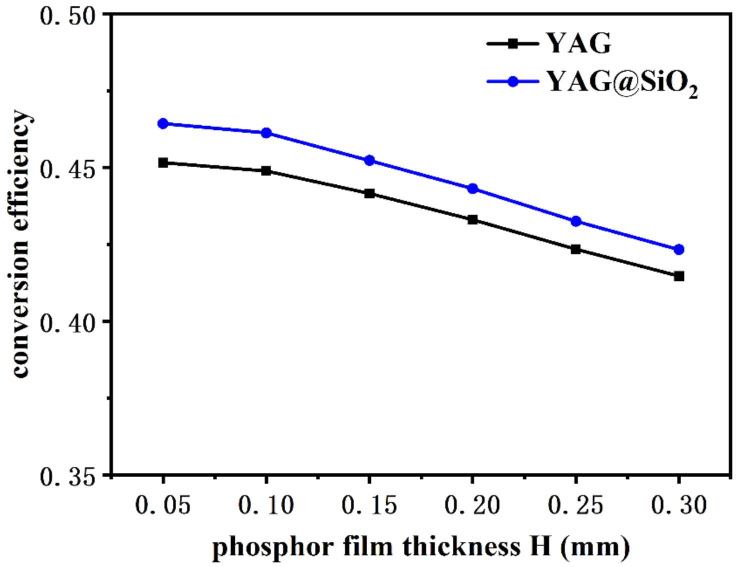


**Fig. 8 Conversion efficiency of phosphor**

Fig. 8 shows the conversion efficiency of YAG and $YAG@SiO_2$ excited by blue LED. As the thickness of the phosphor film increases, the conversion efficiency of phosphor gradually decreases, it might due to the fact that when the film is too thick or the phosphor concentration is too high, the oversaturated phosphor causes more converted light to be back reflected [21], and less light to be forward reflected. This might cause multiple reflection of the converted light between the phosphor layer and the chip. The multiple reflection result in the high absorption of converted light and decrease of luminous efficiency. However, YAG@$SiO_2$ has a 1.2% higher conversion efficiency than YAG, which implies that phosphor coating might be an effective way to improve the light efficiency.

In order to generate white light, the luminescence efficiency and true color map of the CSP WLED with different YAG film thickness ( H ) is simulated. As the thickness of the YAG fluorescent film increases, the luminous efficacy and color temperature of blue LED excited WLED gradually increase. When H is 0.3mm, the luminous efficiency gradually reaches saturation. When H is 0.2mm, the fabricated CSP LED possess a cold white light emission with a CCT of 10066K, color coordinates of (0.2851, 0.2786) ( as shown in Fig.11(b) ) and a luminous efficacy up to 130.3 lm/W (as shown in Fig.9).

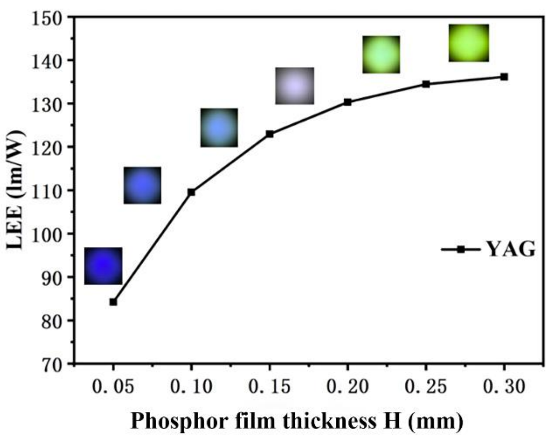


**Fig. 9 Influence of YAG fluorescent film thickness on luminous efficiency of YAG WLED**

The fluorescent film thickness (H) is fixed at 0.2mm, the influence of $SiO_2$ coating thickness on the luminous efficiency (LEE) and Correlate Color Temperature (CCT) of CSP WLED are shown in Fig.10. With the increasing of $SiO_2$ coating thickness, LEE of CSP WLED firstly increase and then decrease. When the coating thickness is 20nm, the luminous efficacy reached the maximum value 138.92 lm/W. This might due to the fact that $460\mu_{abs}$ of YAG@$SiO_2$ phosphor reaches the highest value while the $SiO_2$ coating thickness is 20 nm. Under this condition, more blue light emitted from the chip could be absorbed by YAG@$SiO_2$ phosphor film. More absorption of blue light by the YAG@$SiO_2$ phosphor, more emission of yellow light, therefore enhanced LEE is obtained.

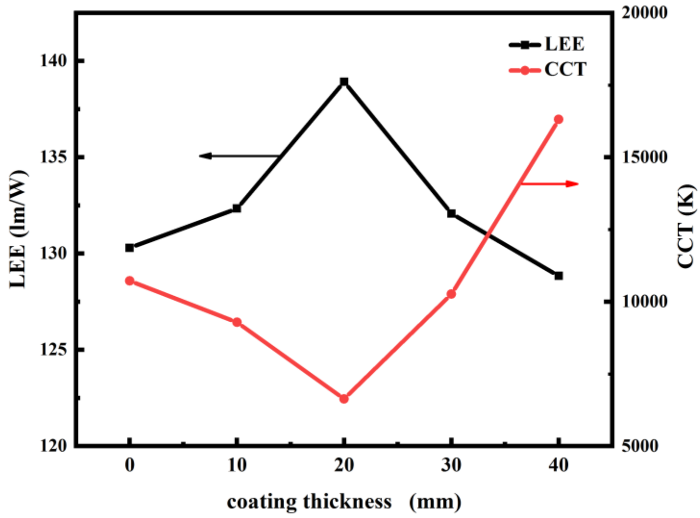


**Fig.10 Influence of coating thickness on LEE and CCT of CSP WLED**

Meanwhile, CCT of YAG@$SiO_2$ WLED decreases when the thickness of $SiO_2$ coating layer increases from 0 to 20 nm. When the thickness of the $SiO_2$ coating layer is over 20 nm, the color temperature of YAG@$SiO_2$ WLED increases sharply. Low color temperature WLED is prefer under working condition. It is found that proper $SiO_2$ layer thickness endowing YAG@$SiO_2$ with more absorption of blue light and high output of yellow light, therefore significantly enhance the LEE and decrease the

CCT of WLED. The highest value of LEE, 138.92 lm/W, the lowest CCT, 6667K, are achieved at a $SiO_2$ layer thickness of 20nm. The simulation results above show that proper $SiO_2$ coating on phosphors is responsible for the enhanced luminous efficacy and lower color temperature of CSP WLED, which is in accordance with the former reports. [23]

Using Monte Carlo method, the quality of white light emission from the YAG and YAG@$SiO_2$ WLED was evaluated via CIE chromaticity diagram and Luminous flux figure (as shown in Fig.11). The results are listed in Table 2.

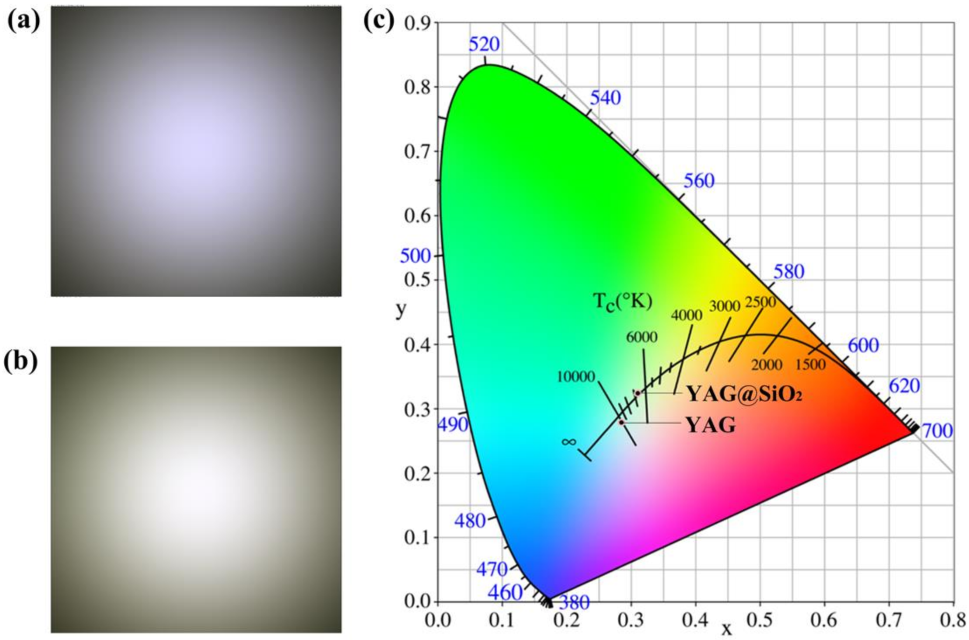


**Fig. 11 (a) Luminous flux figure of YAG WLED; (b)Luminous flux figure of YAG@$SiO_2$WLED; (c) Chromaticity color coordinates of YAG and YAG@$SiO_2$ upon excitation at 460 nm**

**Table. 2 Optical properties of YAG and YAG@$SiO_2$ WLEDs Simulated by Monta Carlo Ray Tracing method**

| Phosphor | LEE (lm/W) | CCT (K) | CIE (x, y) | Fluorescence conversion efficiency |
|---|---|---|---|---|
| YAG | 132.11 | 10066 | (0.2851,0.2786) | 0.4299 |
| YAG@$SiO_2$ | 138.92 | 6637 | (0.3110,0.3244) | 0.4392 |

When the thickness of fluorescent film is 0.2 mm, $SiO_2$ coating layer is 20 nm, YAG@$SiO_2$ WLED shows a light efficiency of 138.92 lm/W, a color temperature of 6637K, and a color coordinate of (0.3110, 0.3244), as shown in Tab.2. Compared with original YAG WLED, higher LEE and lower CCT is achieved in YAG@$SiO_2$ WLED, which is resulted from enhanced forward scattering and stronger blue light absorption. Meanwhile, the color coordinates of YAG@$SiO_2$ WLED is closer to the theoretical white point of (0.33, 0.33). This result shows that an ideal white color is almost achieved in YAG@$SiO_2$ under 460nm blue LED excitation. Meanwhile, proper $SiO_2$ thin layer coating on YAG significantly enhanced LEE and CCT of WLED, and a good cold white light emission is achieved.

Our simulation gives a theoretical explanation about the reason why proper coating thickness on YAG phosphor endows the CSP WLED with higher luminous efficacy and lower color temperature, hence better luminescence properties.

## 5. Conclusions

Optical configuration of chip scale packages WLEDs are established by coating YAG or YAG@$SiO_2$ phosphor film directly on the chip surface. In order to ensure the correct simulation of luminescence properties of the CSP white LED, the specific optical constants including the absorption coefficient $\mu_{abs}$, scattering coefficient $\mu_{sca}$, and anisotropy factor $asy$ of YAG and YAG@$SiO_2$ are calculated based on Mie scattering theory. The dependency of coating thickness of $SiO_2$ layer and phosphor mass fraction $w_f$ on optical constants $\mu_{abs}, \mu_{sca}$ and $asy$ are investigated. It shows that when the coating thickness is 20 nm, the absorption coefficient increases the most, which is conducive to increase the absorption of blue light, enhance the yellow light emission and eventually improve the luminescence property. The decrease in scattering coefficient is also conducive to the improvement of luminous efficiency. Numerical results show that Mie theory is effective in predicting the changing tendencies of the optical constants as the mass fraction of phosphor or the coating thickness changes. It makes Mie theory a suitable tool in WLED packaging design. Two color LEDs are used as light sources to simulate the light extraction of YAG and YAG@$SiO_2$ WLED via Monte Carlo ray tracing method. It implies that $SiO_2$ coating mainly result in the enhanced absorption of blue light and yellow light converting, hence the higher conversion efficiency for YAG@$SiO_2$. As the thickness of the fluorescent film is 0.2 mm, with 2 μm YAG@$SiO_2$ coated by 20 nm $SiO_2$ layer in it, our WLED gives a light efficiency of 138 lm/W, a color temperature of 6637 K, and a color coordinate of (0.3110, 0.3244), The light conversion efficiency after coating is increased by 1.2% compared with that before coating.

The simulation of photoluminescence property of YAG@$SiO_2$ WLED can be adapted to various coated phosphors WLED systems, the color quality can be easily tuned by changing the coating thickness, the phosphor film thickness or the mass fraction of phosphor, which have potential use in the future WLED packaging designing.

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**Declaration of interests**

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Declaration of Interest Statement

We declare that we have no financial and personal relationships with other people or organizations that can inappropriately influence our work, there is no professional or other personal interest of any nature or kind in any product, service and/or company that could be construed as influencing the position presented in, or the review of, the manuscript entitled “Simulation of Optical behavior of YAG:$Ce^{3+}$@$SiO_2$ phosphor used for chip scale packages WLED”.