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Precise Simulation of Spectrum for Green Emitting Phosphors Pumped by a Blue LED Die

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Abstract: This paper proposes an effective approach for spectrum shaping in the optical modeling of phosphor-converted white light-emitting diodes (LEDs) in which overlapping of the absorption and emission spectra of the phosphor are considered. The spectrum shaping method was applied to explore the wavelength-dependent absorption effect and reabsorption by the green phosphor. The experimental results indicated that the adjustment factor for blue light can enable the blue light spectrum to fit well with the measured spectrum. The adjustment factor was linearly related to the transmission ratio of the blue light. The blue light emitted by the blue die and the green light emitted by the phosphor were simulated and predicted in an accurate way as compared with the experimental measurements. The enhanced accuracy in assessing the spectra resulted in enhanced precision of chromaticities. In the experiments, the color differences were one order smaller in CIE 1931 chromaticity ($\Delta x, \Delta y$) than in models without spectrum shaping and were almost imperceptible to the human eye. The novel optical modeling of green phosphor pumped by a blue die facilitates the application of these materials in high-color rendering in white LEDs and projection displays.

Index Terms: Light-emitting diodes, non-imaging optical systems, illumination design, optical design and fabrication, illumination.

1. Introduction

Energy-efficient solid-state lighting has been extensively studied because of the rapid increase in the energy efficiency of white light-emitting diodes (LEDs) [1]. Most white LEDs are manufactured using yellow-emitting phosphors and gallium nitride (GaN) blue dies because such a process is simple and cost effective [2]–[6]. However, in previous studies, the color rendering index (CRI) of white LEDs was approximately 70, failing to meet the requirements for color



Fig. 1. The absorption and emission spectrum of the green YAG phosphor. Note that the absorption spectrum is normalized to its maximal value at 441 nm.

performance [7], [8]. The CRI can be improved by applying two phosphors, such as green and red phosphors, to enhance high-fidelity lighting [9]–[16]. Previous studies have established optical models of yellow-emitting phosphor [17]–[19]. However, no satisfactory optical model applicable to green-emitting phosphor has been developed. The application of blue light in pumping green-emitting phosphor in projection displays has been explored because the insufficient efficiency of green-light sources cannot meet practical demands. Therefore, a model of green-emitting phosphor is required.

Green-emitting phosphor models differ from yellow-emitting phosphor models because the spectrum of the blue light emitted by the LED die and that of the green light emitted by the phosphor partly overlap each other. The distortion of the spectrum in the overlapping part may cause considerable error in evaluating chromatic performance because of reabsorption in the spectrum between the blue light and the peak of the green light. Therefore, an effective and accurate model for simulating the spectrum of green phosphor pumped by a blue die is necessary. This paper proposes a new modeling algorithm whereby spectrum shaping technology is applied to adjust the distorted spectrum in accordance with the model for yellow-emitting phosphor. The corresponding experiments are described.

2. Optical Parameters

The green phosphor used in the study was a cerium-doped yttrium aluminum garnet (YAG:Ce) phosphor $(Y, Tb)_3Al_5O_{12} : Ce^{3+}$, of which the density was 4.3 g/cm³, the emission band was centered at approximately 526 nm, and the particle size approached a Gaussian distribution with a peak at 15 μ m. Fig. 1 shows the absorption and emission spectra. These data were recorded using spectro-fluorimeter SPEX FL212 with a process described in Ref. [20]. The scattering model, absorption coefficient, and conversion efficiency were investigated to model the behavior of the blue light and the reemitted green light in the phosphor volume. The absorption of the volume containing phosphor and silicone is described as

$$I(d) = I_0 e^{-\alpha d} \tag{1}$$

where l_0 is the optical intensity of the incident light, α is the absorption coefficient and *d* is the traveling length of light. The down conversion of the phosphor from the blue light to the green light can be described as

$$I_G = \eta_c \cdot I_{B,abs} \tag{2}$$



Fig. 2. The experimental setup of the measurement of the scattering distribution of the phosphor plates (bottom left side).

where I_G is the intensity of the green light, $I_{B,abs}$ is the absorption intensity of the blue light, and η_c is the conversion efficiency. Once the scattering behavior, absorption coefficient, and conversion efficiency are calculated, Monte Carlo ray tracing with Mie scattering was performed to simulate the output of blue and green light in the volume containing phosphor and silicone incorporated with the incident blue light.

3. Optical Modeling

Optical modeling was conducted based on the procedure used to model yellow-emitting phosphor [17], [18]. The model fit well with corresponding experimental measurements and was used to predict the spectral distribution, efficiency, chromaticity, and angular distribution of any LED device composed of the studied phosphors and blue dies.

The modeling procedure began with scattering simulation conducted using Monte Carlo raytracing software incorporating Mie scattering. Fig. 2 shows the setup of the experiments conducted to measure the scattering light distribution. The phosphor plates used in the experiment had phosphor concentrations of 5%, 7.5%, 10%, and 15% and thicknesses ranging from 0.4 mm to 1.8 mm. The phosphor plate was placed at the rotational center of a rotational stage, and a laser with a wavelength of 632.8 nm was used as the light source. A power meter rotated around the phosphor plate and detected the scattered light. Once all angular distributions of the scattering light for various phosphor plate thickness and concentrations were obtained, simulations were performed by manipulating the refractive index and the particle size of the phosphor until the simulated scattering distribution fit the measurement in the experiment, as shown in Fig. 3. The simulation results effectively describe the spatial light distribution upon Mie scattering. The fitted refractive index is found as 2.1, and the fitted particle size of phosphors is found as 11.2 μ m which is very close to the peak particle size (15.0 μ m) with most probable population in the measured particle size distribution of the phosphors.

The second step involved calculating the absorption coefficient and conversion efficiency. Fig. 4(a) shows the packaging configuration in the measurement and Fig. 4(b) the corresponding structure in simulation. The packaging configuration is consisted of a MCPCB board, a Cree EZ-700 blue LED die with a peak wavelength of 449 nm, a black acrylic plate, and the phosphor plate. Fig. 4(c) demonstrates the consistency in the angular distribution of the light intensity from the measurement and the simulation. The black cavity absorbed the reflected light from the phosphor plate. The simulation of the light pattern of the blue die in the cavity was consistent with the measurements [21]–[23]. The green and blue light transmitted from the phosphor plate was measured after placing the samples in an integrating sphere. Figs. 5 and 6 show the measurements of phosphor plate of various thicknesses and concentrations. In addition, three samples of each type of phosphor plate were studied to prevent deviation errors in the fabrication process and measurements.



Fig. 3. The simulation and the corresponding measurement results of scattering. (a) The schematic diagram, and the concentration of (b) 5%, (c) 7.5%, (d) 10%, and (e) 15%.



Fig. 4. (a) The cavity with blue die in the measurement of blue and green lights, (b) the corresponding structure in simulation, and (c) the simulation and experimental measurement.



Fig. 5. (a) Measurement results of blue light from the phosphor plate and (b) the calculated absorption coefficient.

The measurements shown in Fig. 5(a) were used to determine the absorption coefficient by using (1). The absorption coefficient α is independent of the thickness of the phosphor plate, but is a function of the concentration, as shown in Fig. 5(b). The fitting polynomial of the absorption coefficient versus the concentration is written as

$$\alpha = 0.0733 \times C - 0.0348 \tag{3}$$

where *C* is the weight percent concentration of the phosphor. Equation (3) can be used within the concentration range from 7.5% to 20%.

Fig. 6(a) shows the measurements of green light emitted by the green-emitting phosphor. On the basis of (2), the conversion efficiency was further analyzed as shown in Fig. 6(b). The



Fig. 6. (a) Measurement results of green light from the phosphor plate and (b) the analyzed conversion efficiency based on (2).

results indicated that the conversion efficiency was independent of both the thickness and the concentration of the phosphor plate. According to (2), the average conversion efficiency was 0.7755. In fact, the conversion efficiency is more like the quantum efficiency but counting in energy rather than in photon numbers. Since the conversion efficiency is one of the characteristics of the phosphors, it should be independent of how much the amount of the phosphors are used. So, the conversion efficiency is observed almost independent of thickness and concentration.

According to the modeling algorithm, once the scattering property, absorption coefficients, and conversion efficiency are obtained, the phosphor pumped by the blue die of a specific wavelength can be simulated effectively. The samples were fabricated by attaching a phosphor dome on a GaN die at a peak wavelength of 449 nm. The dimensions of the packaging were carefully measured and applied in the simulation

4. Modified Model With Spectrum Shaping

As shown in Fig. 7(a) and (b), the samples of green-emitting phosphors were prepared in a mixture with silicone and formed a dome under the hemispherical lens to cover the blue GaN dies. All of the samples (7.5%, 10.0%, and 15.0% in concentration) were applied in three verification procedures: the first involved conducting experimental measurements (red solid lines); the second involved summing the blue light spectrum of GaN dies and the emission spectrum of the green-emitting phosphors (blue solid lines); and the third involved conducting optical model simulation (green solid lines). The simulation results obtained from conventional simulation procedures exhibited considerable deviation from the corresponding experimental results [as shown in Fig. 7(c)–(e)]. In addition, the results revealed that the deviation in spectra occurred near the valley between the blue peak and the green band. Furthermore, the blue-die emission model did not fit as well with the measurements as the green-die emission model did.

In principle, the scattering effect is considered in the simple summation method. In the optical model simulation method, the reabsorption effect is also considered. Regarding the featured spectra of the blue light emitted by GaN dies and the green light emitted by green-emitting phosphors, the simulation is simplified because only two wavelengths of the complete spectrum are studied instead of the full-spectrum calculation for the optimal calculation efficiency. First, the spectra of the blue and green lights are regarded as two single lines in the simulation. In this study, the wavelengths of the blue and green lights are obtained, the single lines in the full spectra of blue and green lights are obtained, the single lines in the full spectra of blue and green lights are obtained. The single lines in the full spectra of blue and green lights are obtained. The single lines in the full spectra of blue and green lights are obtained. The single lines in the full spectra of blue and green lights are obtained. The simulation is a linear combination of the weighted blue and green spectra. The simulation is sufficiently accurate in most conventional cases of blue dies used in conjunction with yellow phosphor [17], [18].

However, the resultant spectrum becomes increasingly distorted as the emitting spectrum of phosphors approaches the pumping spectrum of the GaN die. The distortion of the spectrum, especially in the spectral band of the overlap between the blue-pumping and green phosphor emission spectra, can be attributed to the wavelength-dependent absorption of the blue light, as



Fig. 7. (a) The schematic of the packaged LED and (b) a photo of a real sample. Comparison of the spectrum among the linear summation, the optical model simulation, and the corresponding measurement at the phosphor concentration of (c) 7.5%, (d) 10%, and (e) 15%.

shown in Fig. 8(a), and the reabsorption of green light by the green phosphor. Fig. 8(b) shows measurements of the spectra of the blue light at various phosphor concentrations, illustrating that the greater the phosphor concentration or thickness of the phosphor plate is, the more distorted the spectrum becomes.

To adjust the distorted spectrum, the spectrum shaping method was applied in investigating the wavelength-dependent absorption and reabsorption effects. According to the experimental observations, the real output spectrum, $S_{B,o}(\lambda)$, can be obtained using the pumping blue spectrum, $S_{B,i}(\lambda)$, which is adjusted according to a relation expressed as

$$S_{B,o}(\lambda) = S_{B,i}(\lambda) - \beta \times S_{B,i}(\lambda) \times S_{G,abs}(\lambda)$$
(4)

where $S_{G,abs}(\lambda)$ is the absorption spectrum of the green phosphor, and β is an adjustment factor for blue light based on experimental measurement. The relation in (4) enables the complex mechanism of the reabsorption of phosphor emission, emission of phosphor that can be reabsorbed by the green phosphor below 520 nm, and wavelength-dependent absorption to be considered. When the absorption spectrum represents in percentage as usual, the total amount of the blue light absorption must be dependent on the practical quantity of the phosphors applying in the LED packaging, which will make the analysis become more complicated. Here, we utilize the normalized absorption spectrum rather than the conventional one. In this way, the normalized absorption spectrum itself takes response for the wavelength dependency. Meanwhile, the



Fig. 8. (a) Absorption spectrum of the green phosphor and the blue spectrum of the LED die. Note that the absorption spectrum is normalized to its maximal value at 441 nm. (b) The spectra around blue light for different phosphor concentration or different thickness of the phosphor plates.



Fig. 9. The adjustment factor for blue light, β is almost linearly to the transmission ratio τ of the blue light in green phosphor plate.

adjustment factor β is then simply corresponding to the total amount of absorption and thus could be wavelength independent.

Experimental observation indicated that the value of β is not dependent on the wavelength within the blue band of the spectrum, and can enable the blue light simulation spectrum fit to the measured spectrum very well. Unexpectedly, β is almost a linear function of the transmission ratio (τ) of the blue light, as illustrated in Fig. 9, where t is defined as the ratio of the transmission power to the incident pumping power of the blue light in a phosphor plate as shown in (5). Naturally, more the transmission ratio of the blue light is, lesser the absorption of the blue light is, then the factor β decreases

$$\tau \equiv \frac{\int_{360 \text{ nm}}^{520 \text{ nm}} S_{B,o}(\lambda) d\lambda}{\int_{360 \text{ nm}}^{520 \text{ nm}} S_{B,i}(\lambda) d\lambda}.$$
(5)

Actually, the value of β decreases when the transmission ratio of the blue light increases upon passing through the green phosphor plate. Thus, β can be conveniently obtained from the characterization measurements on the phosphor plates in advance as illustrated in Figs. 4–6 instead of the post evaluation on the real diverse packaging samples.

A precise spectrum of a real packaging LED composed of green phosphor covering a blue die then was simulated by employing the spectrum shaping method with β correction. Fig. 10



Fig. 10. The new spectra of the simulations with β correction in comparison with the spectra measured from the corresponding samples with the concentration of (a) 7.5%, (b) 10%, and (c) 15%.

TABLE 1

Color differences (Δ_x , Δ_y) between the simulations with/without β correction and the corresponding measurement on the reals packaging samples

Concentration	7.5%	10%	15%
With β correction	(0.0031,0.0038)	(0.0041,0.0024)	(0.0000,0.0086)
Without β correction	(0.0014,0.0110)	(0.0058,0.0206)	(0.0029,0.0109)

shows the improved spectra of some examples. In addition, the chromatic performance, which was evaluated according to the color difference between the measurements of the real packaging samples and the simulation conducted with or without β correction, is summarized in Table 1 and shown in Fig. 11. In Fig. 11, the arrows indicate color differences, and the heads and tails of the arrows indicate the chromaticity coordinates of the simulation results and the experimental measurements, respectively. The color differences were compared with the one-step and three-step MacAdam ellipses [24], [25]. The color differences in a three-step MacAdam ellipse are almost imperceptible to the human eye.

In summary, the β correction conducting spectrum shaping accounts for the reabsorbed phosphor emission below 520 nm and compensates for the spectrum distortion of the blue light to enable accurate simulation of the packaging containing green phosphor covering a blue die. Thus, the original model of yellow phosphor and a blue die can be further modified by inserting a process of spectrum shaping for β correction as illustrated in Fig. 12. This modified model can be used to predict the emission spectra of all real samples of green phosphor pumped by a blue die more accurately.

5. Conclusion

In this study, an effective and efficient method for spectrum shaping was developed and applied in modifying the simulation of the spectra of green phosphor pumped by a blue die. Application of spectrum shaping in the optical modeling of phosphor-converted white LEDs was proposed. A new adjusting parameter was implemented to correspond for the overlap of the absorption and emission spectra of phosphor. As a result, an emission light with a spectrum close to the pumping spectrum can be predicted effectively simply by simulation.



Fig. 11. Color differences shown in CIE 1931 chromaticity diagram and are compared with 1-step and 3-step MacAdam Ellipses. All the heads and the tails of the arrows are the chromaticities from the simulation results and the experimental results, respectively. The blue ones represent the cases after the β correction and the red ones denote the cases before the β correction.



Fig. 12. A modified phosphor modeling procedure for a green phosphor with a blue die, where the introduction of β is different from the old one.

All experiments revealed that the spectrum shaping method applied in the optical simulation model exhibited high accuracy. The green phosphor used in the study was a YAG phosphor: $(Y, Tb)_3Al_5O_{12} : Ce^{3+}$. Two crucial parameters, the absorption coefficient and conversion efficiency, were integrated and combined with the scattering model. Spectrum shaping was employed to explore for the wavelength-dependent absorption effect and reabsorption by the green phosphor. In addition, the adjustment factor β for blue light was easily evaluated from characterization measurement in advance. Experimental observation indicated that an appropriate β can enable the blue light spectrum to fit to the measured spectrum very well. Empirically, the value of β linearly decreases when the transmission ratio of the blue light increases upon passing through the green phosphor plate.

The blue light emitted from the blue LEDs with pumping the green phosphors can thus be predicted in simulation and achieve high accuracy as compared with the experimental measurements. In the study, the thickness of the green phosphor plate varied from 0.6 mm to 1.8 mm, and the concentration ranged from 7.5 wt% to 15.0 wt%. The enhanced accuracy in assessing the spectra resulted in the enhancement on the precision of chromaticities, too. Within the scope of our experiments on the test samples, the color differences with beta correction become insignificant. As represented by the CIE 1931 x-y chromaticity coordinates, the color differences ($\Delta x, \Delta y$) are reduced to as small as (0.0031, 0.0038) at 7.5 wt%, (0.0041, 0.0024) at 10.0 wt%, and (0.0000, 0.0086) at 15.0 wt%. These small color differences (less than those of a three-step MacAdam ellipse) are almost imperceptible to the human eye. An accurate optical model of green phosphor pumped by a blue die was thus developed. The modeling algorithm can facilitate high color rendering in white LEDs and optical projectors.

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