High-accuracy emission modeling of yellow phosphor YAG: Ce validated by normalized cross-correlation

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Abstract—The yellow phosphor YAG:Ce3+ emission shows an asymmetric shape that causes the difficulty of spectrum modeling. We proposed and demonstrated a method for modeling the emission of yellow phosphor $YAG:Ce^{3+}$. The mathematical model is developed based on the Gaussian function. The model's accuracy is quantitatively verified by comparing the simulation and experimental results. Normalized cross-correlation algorithms were applied to quantitatively define the similar level between the simulation and experiment results. The proposed model is helpful for emission spectrum modeling and efficient for studying the optical properties of yellow phosphor.

Light-emitting diodes (LED) based on solid-state lighting have become the dominant light source due to their advantages of energy saving, compact size, luminous efficiency, and being environmentally friendly [1, 2]. The yellow phosphor YAG: Ce3+ has been widely used in manufacturing white light due to its unique properties, such as its broad emission band (wavelength range from 500 nm to 750 nm). In combination with the blue light of the excitation light source, the white light can easily generated under the perception of human eyes for the generated light mixture that includes transmitted light and converted yellow light [2]. Figure 1 illustrates the white light generation from the combination of yellow phosphor and blue light excitation sources.

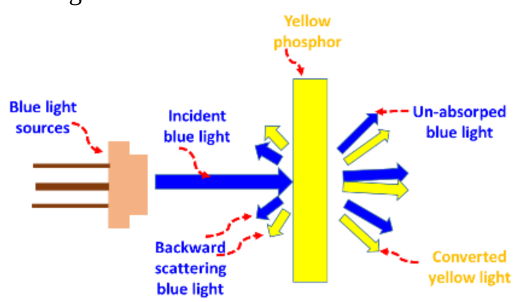

Fig. 1. White light generation through a combination of yellow phosphor material and blue light excitation sources.

The optical property of this light mixture is controlled by changing the power ratios of blue and yellow light. In the packaging process for white light, many phosphor-related phenomena need to be considered to obtain the highest output light efficiency and quality for the overall light source package module [2-4]. Optical modeling is an important technique to optimize the factor (e.g., phosphor weight concentration, color error, correlated color temperature value) to generate the output white light with the highest optical and color performance [3-10]. However, there is a disadvantage in its emission spectrum that usually causes difficulty when matching the emission between the simulation and experimental spectrums. The asymmetry characteristic of the emission spectrum of yellow phosphor can be shown in Fig. 2. This emission band originated from the band structure transitions related to the down conversion contributions in the energy range due to the spin-orbit coupling effect between the $(5s^25p^6)\ 5d^1$ excited state and $(5s^25p^6)\ 4f^{one}$ ground state [11]. The higher the radiative recombination has happened, the stronger the intensity of the emission band is obtained.

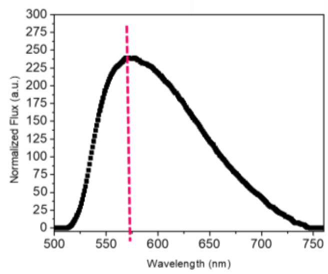

Fig. 2. The asymmetry characteristic of the emission spectrum of yellow phosphor.

In this study, we proposed and demonstrated a solution to solve the difficulty related to the asymmetry characteristic of the emission spectrum of yellow phosphor $(YAG:Ce^{3+})$. The emission spectrum is analyzed into two halves with different full widths at half maximum (FWHM) values, and based on the mathematical model developed based on the Gaussian function, the emission spectrum can be modeled efficiently. The accuracy of the proposed solution is quantitatively verified by comparing the simulation and experimental results.

The principle for modeling the un-symmetry emission band started from the characteristics of the

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curves, which can de-convolute the band into two parts corresponding to two emission bands having different FWHM. Figure 3 illustrates the analysis of the emission spectrum into two halves. The modeling for each half is independently conducted.

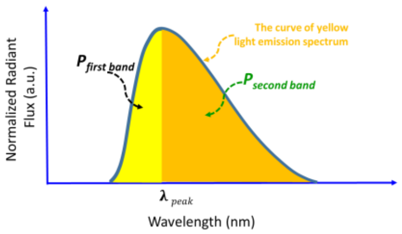

Fig. 3. Illustration of analyzing the asymmetry emission spectrum into two halves.

In terms of mathematical modeling, the emission spectrum with the radiant power of P_{total} can be written as:

$$P_{total}(\lambda) = P_{first\ band}(\lambda) + P_{second\ band}(\lambda), \tag{1}$$

where $P_{first\ band}(\lambda)$ and $P_{second\ band}(\lambda)$ are the radiant power for each half contributing to the total emission spectrum. $P_{first\ band}(\lambda)$ and $P_{second\ band}(\lambda)$, can described by the function [12].

$$P(\lambda) = P\ exp\left[-\beta\left(\frac{\lambda - \lambda_{peak}}{\Delta E}\right)^2\right] \tag{2}$$

where β is the corrected coefficient, ΔE is the FWHM in nm, and P is the optical power of LED.

According to Eq. (2), some parameters are constant while others are not. These variable constants should be optimized to ensure the highest matching level between the simulated and the experimental spectrum. Based on the principle for modeling as described above and the experimental emission spectrum, these parameters are obtained: Yellow light emission range of wavelength from 475 nm to 850 nm, emission Peak is 575 nm, the width for two halves are FWHM equals 74 nm (from 538 nm to 575 nm) for the first half and FWHM of 154 nm (from 575 nm to 652 nm) for the second half, respectively. There is still a β parameter that needs to be defined. It thus required an investigation process to determine the optimal β value so that its simulation spectrum would match the experimental spectrum at the best level. In addition, it can visualize the shape of the emission band in the simulated spectrum corresponding to the β value. Different β values, including 1.5, 2.5, 3.5, 4.5, 5.5, and 6.5, respectively, were used in the simulation. Figure 4 shows the effect of the β constant on the simulated emission spectrum.

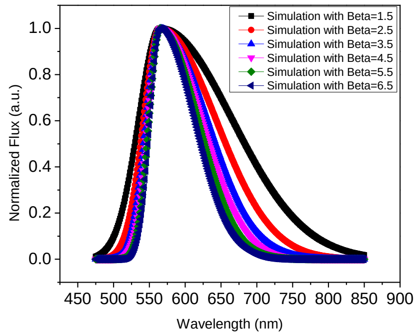

Fig. 4. Effect of β value on the shape of simulation spectrum.

It is essential to find out the value of the β constant to have the best match between simulation and experiment results. For that purpose, different values of the β constant were used in the simulation to simulate the corresponding emission spectrum. Then, this simulated spectrum is compared to the experimental spectrum by overlaps plotting in the exact figure. In qualitative research, the matching level is easily evaluated through the overlap level of two curves. Figure 5 shows the comparison results of the simulation emission spectrum of yellow light at different β values (e.g., 1.5, 2.0, 2.5, 2.8, 3.0, and 3.5) and the experimental emission spectrum of yellow light. In qualitative evaluation, it can be seen that some β values of 2.8, 3.0, and 3.5, respectively, show a high overlap level between the two emission curves.

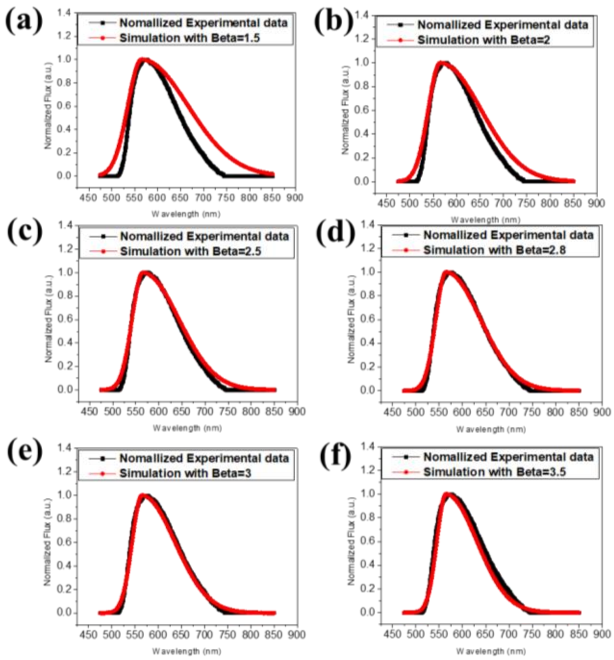

Fig. 5. Comparison between simulation at different values of β and experiment spectrum.

After qualitative evaluation, the β value has the highest level of overlapping of the simulated and experimental spectrum. The precise comparison is conducted through quantitative evaluation using the normalized cross-correlation (NCC) algorithm [8]. The similarity between simulation and experiment spectrum curves is quantitive and evaluated based on the value of NCC (e.g., the value of 100 for NCC means the complete similarity between the simulated and experimental spectrum). In terms of mathematics, the algorithm NCC is expressed as follows:

$$NCC = \frac{\sum_n (S_{\lambda n} - \bar{S})(E_{\lambda n} - \bar{E})}{\sqrt{(\sum_n (S_{\lambda n} - \bar{S})^2)(\sum_n (E_{\lambda n} - \bar{E})^2)}} \quad (3)$$

where $\bar{S}$, $\bar{E}$ are the mean values of the radiant power per unit of wavelength for simulation and experiment spectrum curves that are under comparison, respectively. $S_{\lambda n}$, $E_{\lambda n}$ are the values of the light power per unit of wavelength having a wavelength at the wavelength of the ordering of n for simulation and experiment spectrum curves that are under comparison, respectively.

Applying Eq. (3), the simulated spectrum at different β values is correspondently compared to the experimental spectrum. The corresponding NCC value will be recorded, and the behavior of NCC is shown in Fig.6. The highest NCC value is β equals 2.8. The NCC value corresponding to this obtained optimal β is 99.85.

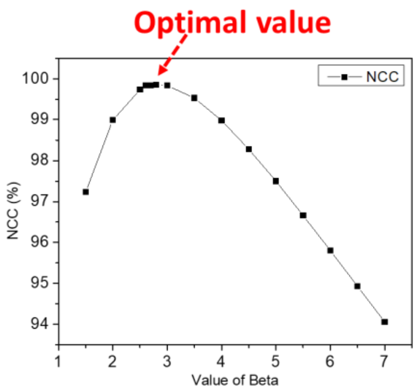

Fig. 6. Changing of NCC versus different values of β.

In summary, origin from the difficulty of spectrum modeling caused by the asymmetry in the emission spectrum of yellow phosphor, we have successfully developed an optical model for the yellow light mission of yellow phosphor pumped by blue light excitation source with the accuracy verified by a normalized cross-correlation algorithm to reach the highest level of similarity between simulation and experiment.

The principle for modeling the un-symmetry emission band is to de-convolute the band into two parts corresponding to two emission bands having different FWHM, then apply the emission modeling based on the Gaussian functions. The proposed modeling has effectively visualized the β value's effect on the emission band's geometrical shape. The shape of the emission band depends on the β value; the more significant the β value is, the narrower the bandwidth of the emission band is.

The optimal value for the β, which has the highest matching level between the simulation and experiment spectrum for the yellow emission band, is 2.8. The NCC value of 99.85 obtained for the optical simulation spectrum compared to the experimental spectrum indicated the high precision of the proposed optical model.

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