

Numerical Investigation of Fe_2O_3 Scattering Particles for Optical Performance Optimization of 4000 K Phosphor-Converted White LEDs

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Abstract—

Phosphor-converted white light-emitting diodes (pc-WLEDs) require an appropriate balance between luminous output and color uniformity to achieve high-quality white light performance. Light scattering within the phosphor layer plays an important role in redistributing emitted photons and consequently affects the angular color characteristics and optical output of the device. In this study, Fe_2O_3 particles were numerically investigated as scattering particles in a 4000 K phosphor-converted white LED over a concentration range of 2–16 wt.%. The optical behavior of the particles was evaluated through their scattering coefficient, reduced scattering coefficient, and particle number density, followed by an analysis of the resulting CCT, ΔCCT , lumen output, color quality scale (CQS), color rendering index (CRI), and spectral power distribution. The simulation results show that increasing the Fe_2O_3 concentration enhances the scattering response and substantially modifies the angular distribution of the emitted light. The CCT exhibits concentration-dependent angular variations, while the ΔCCT indicates that an intermediate Fe_2O_3 concentration provides improved color uniformity. In contrast, the lumen output decreases progressively with increasing Fe_2O_3 concentration. The CQS shows a slight improvement, whereas the CRI exhibits a gradual decrease. These results demonstrate that Fe_2O_3 concentration provides an effective means of controlling the scattering characteristics and color performance of pc-WLEDs, although a trade-off exists between color uniformity and luminous efficiency. The numerical results provide useful guidance for optimizing Fe_2O_3 scattering particles in phosphor-converted white LED systems.

Keywords— Fe_2O_3 ; scattering particles; phosphor-converted white LED; Mie scattering; color uniformity; CCT; CQS; CRI; lumen output

I. INTRODUCTION

White light-emitting diodes (WLEDs) have become an important solid-state lighting technology because of their high energy efficiency, long operating lifetime, compact structure, and flexible optical characteristics [1, 2]. Among the different approaches for producing white light, phosphor-converted white light-emitting diodes (pc-WLEDs), particularly those based on a blue LED chip combined with a yellow-emitting $\text{YAG}:\text{Ce}^{3+}$ phosphor [3, 4], have received considerable attention because of their relatively simple device configuration and practical implementation. However, the optical performance of pc-WLEDs depends strongly on the interaction between the excitation light, phosphor layer, and surrounding optical media. In particular, the spatial distribution of emitted light can vary with observation angle, resulting in non-uniform correlated color temperature (CCT) and consequently affecting the perceived quality of white light [5-8].

Light scattering is one of the important optical mechanisms governing photon propagation inside a phosphor-converted layer. When light encounters particles whose refractive index differs from that of the surrounding medium, the incident photons can be redirected through scattering events. The magnitude and angular characteristics of scattering depend on several parameters, including particle concentration, particle size, refractive index, and wavelength. Therefore, the appropriate selection of scattering particles can provide an

additional means of controlling photon transport and modifying the spatial color characteristics of pc-WLEDs [9-11].

Iron oxide is an attractive class of oxide materials because of its relatively low cost and diverse physical and chemical properties. Several iron oxide phases occur naturally, including hematite ($\alpha\text{-Fe}_2\text{O}_3$), magnetite (Fe_3O_4), and maghemite ($\gamma\text{-Fe}_2\text{O}_3$). Among them, hematite is a thermodynamically stable iron oxide phase and has been investigated for a variety of technological applications. Previous research has demonstrated that Fe_2O_3 can be prepared in nanoparticle form and characterized in terms of its structural, morphological, and optical properties. In particular, Fe_2O_3 nanoparticles have been reported to exhibit characteristic optical absorption behavior in the visible region, indicating that their interaction with light is strongly wavelength dependent [12].

The particle characteristics of Fe_2O_3 are also important when considering its interaction with electromagnetic radiation. Previous experimental characterization of Fe_2O_3 nanoparticles has demonstrated nanoscale particle dimensions together with particle agglomeration and a relatively broad particle-size distribution. For Fe_2O_3 and Ce-doped Fe_2O_3 investigated in the previous study, the reported particle sizes were approximately 132.8 ± 15.8 nm and 21.7 ± 6.7 nm, respectively. Such observations demonstrate that the physical characteristics of iron oxide particles can vary significantly depending on the preparation and composition of the material [13, 14].

Although Fe_2O_3 nanoparticles have been extensively investigated in areas such as catalysis, environmental applications, and biological applications, the optical scattering behavior of Fe_2O_3 particles can also be considered from the perspective of solid-state lighting. The previous Fe_2O_3 study primarily focused on synthesis, structural and morphological characterization, optical absorption, and antimicrobial performance rather than photon scattering in phosphor-converted LEDs. Therefore, the effect of Fe_2O_3 concentration on the scattering characteristics and color performance of a pc-WLED remains an interesting problem for numerical investigation [15].

In a phosphor-converted LED, increasing the concentration of scattering particles can modify the probability of photon-particle interactions and consequently change the propagation path of both excitation and converted photons. The resulting redistribution of optical energy can influence the angular CCT distribution, color uniformity, luminous output, and color-rendering characteristics of the device. However, increasing the scattering strength does not necessarily improve every optical parameter simultaneously. Excessive scattering may increase photon redistribution while also increasing optical losses or extending photon propagation paths, potentially reducing the total luminous output. Thus, an appropriate concentration range must be identified by considering multiple optical performance parameters simultaneously [16].

In this work, Fe_2O_3 particles are investigated as scattering components in a 4000 K phosphor-converted white LED using a numerical optical simulation approach. The Fe_2O_3 concentration is varied from 2 to 16 wt.% to systematically examine its influence on photon scattering and the resulting optical performance. The scattering coefficient, reduced scattering coefficient, and particle number density are first analyzed to establish the relationship between Fe_2O_3 concentration and the scattering behavior of the system. The effect of this scattering modification on the angular correlated color temperature is then evaluated. In addition, the color-temperature deviation (ΔCCT), lumen output, color quality scale (CQS), color rendering index (CRI), and spectral power distribution are investigated to provide a comprehensive assessment of the optical response [17].

The main objective of this study is therefore to establish the relationship between Fe_2O_3 concentration, scattering characteristics, and the optical performance of a 4000 K pc-WLED. By combining scattering analysis with colorimetric and photometric parameters, this study aims to identify the concentration range that provides a reasonable balance between color uniformity and luminous performance. The results are expected to provide a numerical basis for evaluating Fe_2O_3 as a scattering material for optical optimization of phosphor-converted white LED systems.

II. SIMULATION METHOD

A. Numerical Model and Simulation Procedure

A numerical model of a phosphor-converted white light-emitting diode (pc-WLED) was established to investigate the influence of Fe_2O_3 scattering particles on the optical performance of the device. The model consists of a blue-emitting LED, a phosphor layer containing YAG:Ce³⁺ phosphor, and Fe_2O_3 particles serving as scattering centers. The

Fe_2O_3 concentration was varied from 2 to 16 wt.% to evaluate its influence on photon propagation, angular color characteristics, luminous output, and color quality.

For each Fe_2O_3 concentration, the YAG:Ce³⁺ phosphor concentration was adjusted as a color-balancing parameter to obtain a 4000 K-class white-light condition. This adjustment was performed to account for the change in the optical path and spectral contribution caused by the introduction of Fe_2O_3 particles. Therefore, the variation in YAG:Ce³⁺ concentration in the simulation should not be interpreted as a direct chemical or physical reduction of the phosphor by Fe_2O_3 . Instead, it represents the phosphor concentration required to compensate for the optical changes associated with different Fe_2O_3 concentrations.

The simulation procedure was performed by first evaluating the scattering characteristics associated with different Fe_2O_3 concentrations. The resulting scattering behavior was then considered in the photon-transport analysis of the pc-WLED. The simulated optical output was subsequently used to determine the angular correlated color temperature (CCT), CCT deviation (ΔCCT), luminous output, color quality scale (CQS), color rendering index (CRI), and spectral power distribution (SPD). This procedure enables the influence of Fe_2O_3 concentration to be evaluated from both scattering and device-performance perspectives.

The Fe_2O_3 material considered in this study is based on iron oxide with the optical and material characteristics described in the reference study. The reference work provides information on the formation and characteristics of Fe_2O_3 ; however, its experimentally measured particle characteristics are not directly assumed as numerical parameters in the present WLED model unless explicitly specified by the simulation data. This approach avoids introducing unsupported material parameters into the numerical analysis.

B. Scattering Model of Fe_2O_3 Particles

The scattering behavior of Fe_2O_3 particles was described using Mie scattering theory, which is applicable to the interaction between electromagnetic radiation and spherical particles. The size parameter of a particle can be expressed as [18]:

$$x = \frac{2\pi n_m r}{\lambda}, \quad (1)$$

where n_m is the refractive index of the surrounding medium, r is the particle radius, and λ is the wavelength of the incident light.

The scattering cross-section of an individual particle is given by [19]:

$$C_{sca} = Q_{sca} \pi r^2, \quad (2)$$

where Q_{sca} represents the scattering efficiency. For a particle population with a size distribution $N(r)$, the wavelength-dependent scattering coefficient can be expressed as [20]:

$$\mu_{sca}(\lambda) = \int N(r)C_{sca}(r, \lambda)dr. \quad (3)$$

For a discretized particle-size distribution, this relationship can be written as:

$$\mu_{sca}(\lambda) = \sum_i N_i C_{sca,i}(\lambda), \quad (4)$$

where N_i is the number density associated with the i -th particle-size interval and $C_{sca,i}$ is its corresponding scattering cross-section.

The scattering coefficient represents the overall probability of scattering within the phosphor layer and is therefore an important parameter for describing photon propagation. In addition, the reduced scattering coefficient was considered to account for the directional characteristics of scattering. It is defined as:

$$\mu'_{sca} = \mu_{sca}(1 - g), \quad (5)$$

where g is the anisotropy factor, defined as the average cosine of the scattering angle:

$$g = \langle \cos \theta \rangle. \quad (6)$$

A larger value of g indicates a stronger forward-scattering tendency, whereas a smaller value corresponds to a more isotropic scattering distribution. Consequently, the reduced scattering coefficient provides information about the effective scattering strength during photon transport rather than simply describing the total number of scattering events.

The Fe_2O_3 concentration also affects the particle number density within the phosphor layer. Increasing the concentration generally introduces more scattering centers, thereby modifying the probability that photons undergo scattering before exiting the device. The combined consideration of particle number density, scattering coefficient, and reduced scattering coefficient provides a basis for interpreting the changes in optical performance observed at different Fe_2O_3 concentrations.

It should be noted that the particle characteristics reported in the reference Fe_2O_3 study are used only to support the material background of Fe_2O_3 . They are not automatically treated as the particle-size or optical-constant inputs of the present WLED simulation unless such values are explicitly available in the simulation model.

C. Optical Performance Evaluation

The optical performance of the simulated pc-WLEDs was evaluated using angular CCT, ΔCCT , luminous output, CQS, CRI, and SPD. These parameters were selected to provide a comprehensive assessment of the effects of Fe_2O_3 scattering on both color uniformity and luminous/color quality.

The CCT was evaluated from the simulated spectral output at different observation angles. The angular variation in CCT

reflects changes in the relative contributions of blue LED emission and yellow YAG:Ce^{3+} emission as photons propagate through the phosphor layer. The CCT deviation was calculated as:

$$\Delta\text{CCT} = \text{CCT}_{\max} - \text{CCT}_{\min}, \quad (7)$$

where $\text{CCT}_{\max}$ and $\text{CCT}_{\min}$ are the maximum and minimum CCT values obtained over the investigated angular range. A smaller ΔCCT indicates better angular color uniformity.

The luminous output was evaluated from the simulated spectral radiation by considering the photopic response of the human eye. This parameter was used to examine the influence of Fe_2O_3 -induced scattering on the optical efficiency of the pc-WLED. Although stronger scattering can modify the angular distribution of emitted light, excessive scattering can also increase photon path lengths and the probability of optical losses. Therefore, the luminous output was analyzed together with the color-uniformity results rather than considering scattering strength alone as an indicator of improved performance.

Color quality was evaluated using both CQS and CRI. CQS provides an overall assessment of color quality based on multiple color samples, whereas CRI evaluates color-rendering performance using the conventional color-rendering framework. These two parameters were therefore treated as complementary but distinct indicators of the color performance of the simulated WLEDs.

Finally, the spectral power distribution was analyzed to identify changes in the spectral characteristics of the emitted white light. The SPD provides the basis for interpreting variations in CCT, luminous output, CQS, and CRI because changes in photon scattering and YAG:Ce^{3+} concentration can modify the relative spectral contributions of the blue and yellow emission components.

Overall, the numerical analysis follows the relationship:

$$\begin{aligned} &\text{Fe}_2\text{O}_3 \text{ concentration} \rightarrow \text{particle number density} \\ &\rightarrow \text{scattering characteristics} \rightarrow \text{photon transport} \\ &\rightarrow \text{spectral output} \rightarrow \text{CCT}, \Delta\text{CCT}, \text{lumen}, \text{CQS}, \text{and CRI}. \end{aligned} \quad (8)$$

This framework allows the optical effects of Fe_2O_3 scattering particles to be evaluated systematically while considering the trade-off between angular color uniformity, luminous efficiency, and color quality.

III. RESULTS AND DISCUSSION

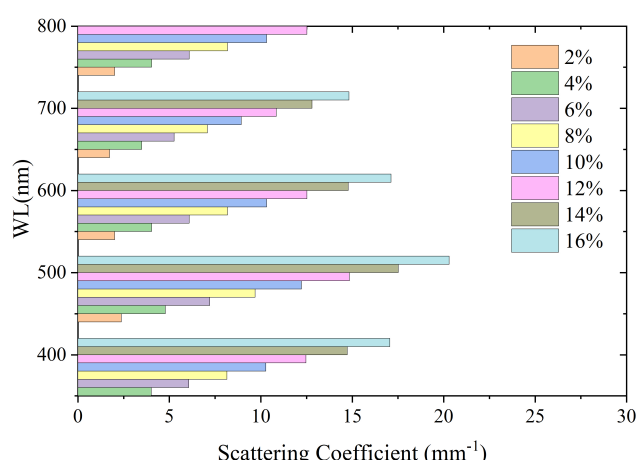
A. Scattering characteristics and phosphor concentration

Figure 1 presents the scattering characteristics of Fe_2O_3 particles, including the scattering coefficient, reduced scattering coefficient, and particle number density. These parameters describe the changes in the optical scattering behavior of the pc-WLED as the Fe_2O_3 concentration varies from 2 to 16 wt.%.

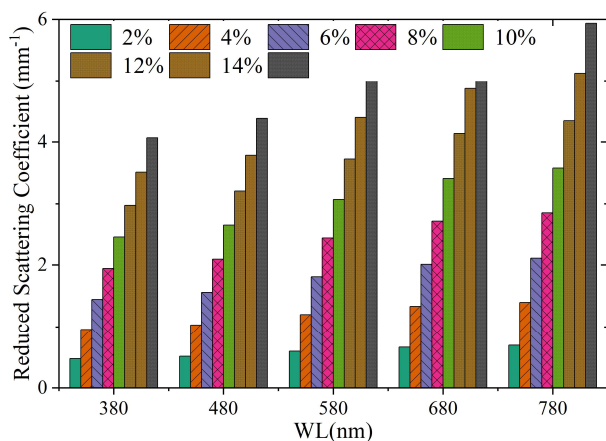
As shown in Figure 1(a), the scattering coefficient changes with increasing Fe_2O_3 concentration, indicating that the

introduction of Fe_2O_3 modifies the interaction between the propagating photons and scattering particles. This behavior is associated with the increasing contribution of Fe_2O_3 scattering centers to the optical system. The scattering coefficient is determined by both the scattering cross-section of individual particles and their number density.

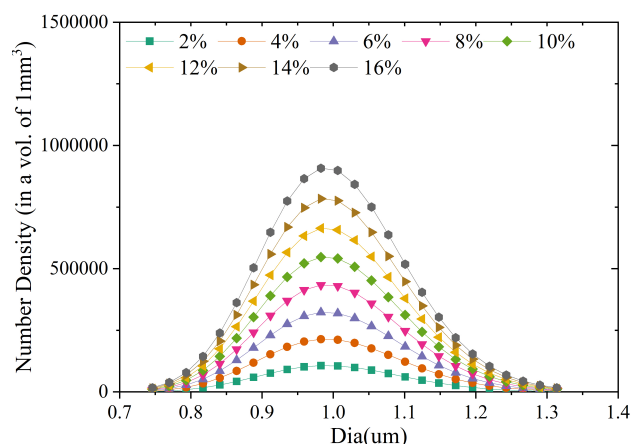
The reduced scattering coefficient in Figure 1(b) exhibits a corresponding variation. Unlike the scattering coefficient, the reduced scattering coefficient also considers the directional characteristics of scattering through the anisotropy factor. Therefore, it provides additional information about the effective transport of photons within the phosphor system. The particle number density shown in Figure 1(c) further explains the change in scattering behavior as the Fe_2O_3 concentration is varied.



(a)



(b)



(c)

Fig. 1. Scattering characteristics of Fe_2O_3 particles at different concentrations: (a) scattering coefficient, (b) reduced scattering coefficient, and (c) particle number density.

The relationship between Fe_2O_3 and $\text{YAG}:\text{Ce}^{3+}$ concentrations is shown in Figure 2. The $\text{YAG}:\text{Ce}^{3+}$ concentration was adjusted for different Fe_2O_3 concentrations to obtain the desired 4000 K-class white-light condition. Therefore, the variation shown in Figure 2 should be regarded as a numerical color-balancing procedure rather than a direct physical effect of Fe_2O_3 on $\text{YAG}:\text{Ce}^{3+}$. The combined results of Figures 1 and 2 indicate that Fe_2O_3 concentration affects the scattering characteristics of the system, while the $\text{YAG}:\text{Ce}^{3+}$ concentration is adjusted to compensate for the resulting changes in the optical and spectral balance.

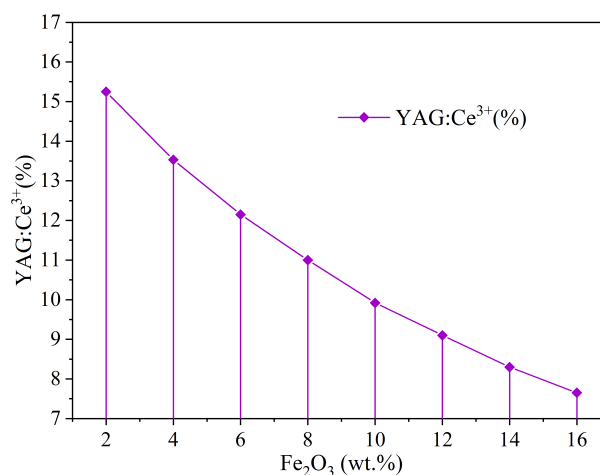


Fig. 2. Variation of $\text{YAG}:\text{Ce}^{3+}$ phosphor concentration with Fe_2O_3 concentration for the 4000 K-class pc-WLED.

B. Angular color characteristics and luminous performance

The angular CCT distributions for different Fe_2O_3 concentrations are presented in Figure 3. The results demonstrate that Fe_2O_3 concentration affects the angular distribution of the emitted white light. This behavior can be attributed to the modification of photon propagation caused by scattering within the phosphor system.

The scattering of blue and phosphor-converted photons changes their propagation paths and consequently modifies their relative contributions at different observation angles. With an appropriate Fe_2O_3 concentration, the redistribution of optical radiation can reduce the difference in spectral composition between different directions. This effect is reflected in the angular CCT profiles shown in Figure 3.

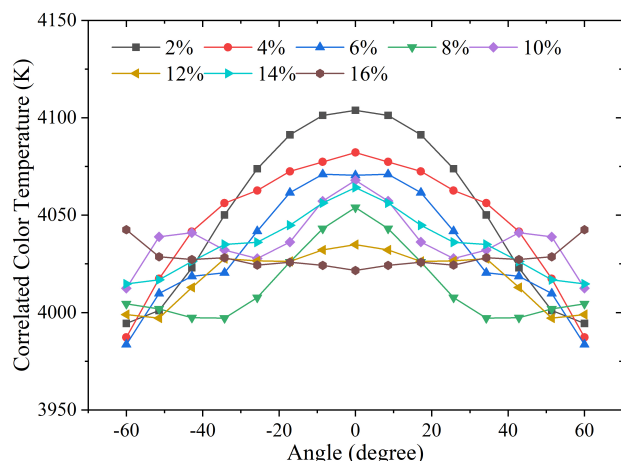


Fig. 3. Angular distribution of correlated color temperature (CCT) for the pc-WLEDs with different Fe_2O_3 concentrations.

The corresponding ΔCCT values are presented in Figure 4. A smaller ΔCCT indicates a smaller angular variation in CCT and therefore better angular color uniformity. The results demonstrate that the Fe_2O_3 concentration plays an important role in controlling the angular color characteristics of the pc-WLED.

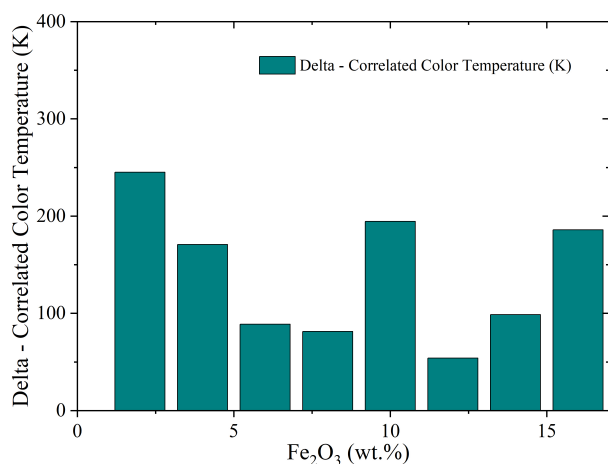


Fig. 4. CCT deviation (ΔCCT) of the pc-WLEDs as a function of Fe_2O_3 concentration.

However, the improvement in angular color uniformity is accompanied by a change in luminous output, as shown in Figure 5. The luminous output decreases as the Fe_2O_3 concentration increases. This behavior can be associated with the increased scattering interaction experienced by photons. Although scattering can redistribute optical radiation and improve angular uniformity, excessive scattering can increase the optical path and the probability of photon loss.

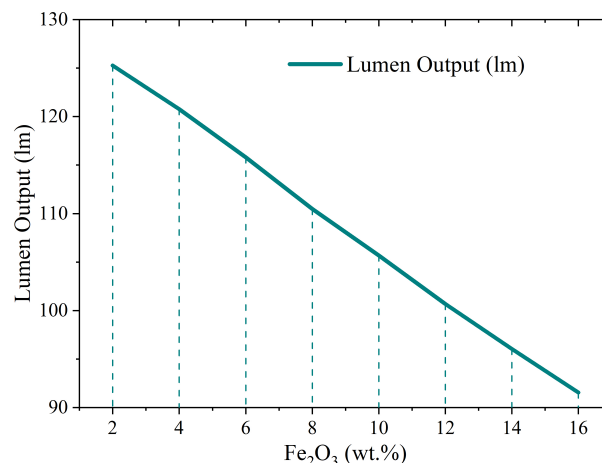


Fig. 5. Luminous output of the pc-WLEDs with different Fe_2O_3 concentrations.

These results demonstrate an important trade-off between color uniformity and luminous efficiency. Therefore, increasing the Fe_2O_3 concentration cannot be considered an unlimited approach for improving the angular color performance of the WLED.

C. Color quality and spectral characteristics

The CQS and CRI results are shown in Figures 6 and 7, respectively. The variation of CQS with Fe_2O_3 concentration indicates that the scattering particles can also influence the overall color quality of the emitted white light. This behavior is related to the changes in spectral composition resulting from the combined effects of Fe_2O_3 scattering and $\text{YAG}:\text{Ce}^{3+}$ concentration adjustment.

The CRI results in Figure 7 provide an additional evaluation of the color-rendering characteristics. Since CQS and CRI are based on different evaluation approaches, their trends should be considered separately rather than assuming that an improvement in one parameter necessarily results in an equivalent improvement in the other.

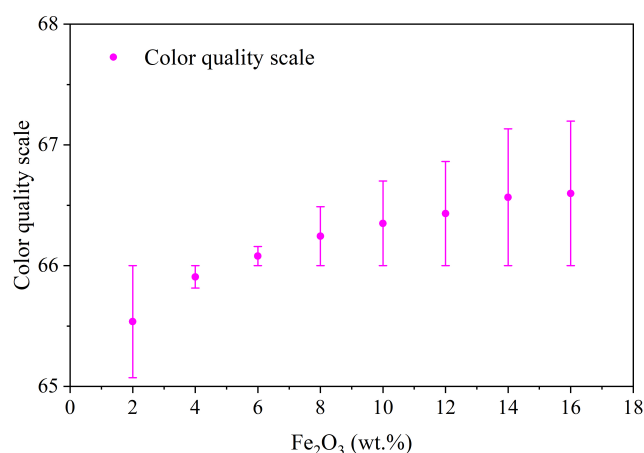


Fig. 6. Color quality scale (CQS) of the pc-WLEDs as a function of Fe_2O_3 concentration.

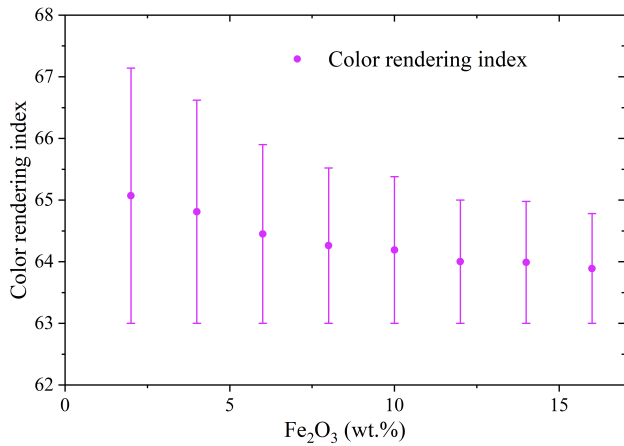


Fig. 7. Color rendering index (CRI) of the pc-WLEDs with different Fe₂O₃ concentrations.

The spectral power distributions shown in Figure 8 provide further insight into these changes. The emitted spectrum contains contributions from the blue LED and the longer-wavelength emission generated by YAG:Ce³⁺. Variation in Fe₂O₃ concentration modifies photon propagation and scattering, thereby affecting the relative spectral contribution reaching the observation direction. These spectral changes are directly related to the variations in CCT, luminous output, CQS, and CRI.

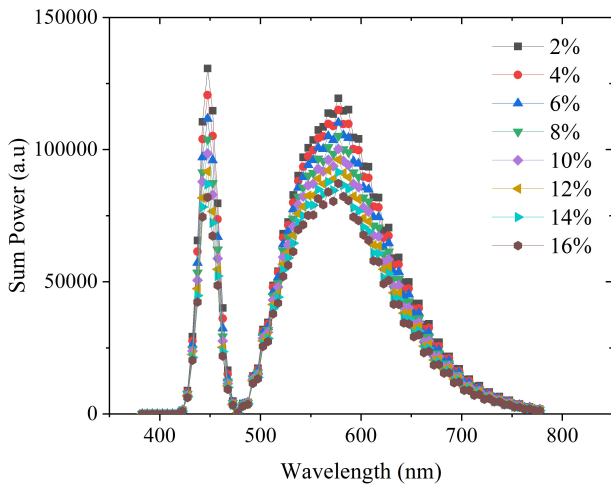


Fig. 8. Spectral power distributions of the pc-WLEDs with different Fe₂O₃ concentrations.

Overall, the results indicate that Fe₂O₃ concentration influences the pc-WLED through a coupled scattering–spectral mechanism. Increasing Fe₂O₃ modifies photon transport and angular color distribution, while the corresponding adjustment of YAG:Ce³⁺ maintains the desired 4000 K-class condition. At the same time, excessive scattering results in a reduction in luminous output. Therefore, the performance of Fe₂O₃-based pc-WLEDs should be evaluated by considering angular color uniformity, luminous output, and color quality simultaneously, rather than using the scattering strength as the sole optimization criterion.

IV. CONCLUSION

This study numerically investigated the effects of Fe₂O₃ scattering particles on the optical performance of 4000 K-class phosphor-converted white LEDs. By varying the Fe₂O₃ concentration from 2 to 16 wt.%, the relationships among scattering characteristics, YAG:Ce³⁺ phosphor concentration, angular color uniformity, luminous output, and color quality were systematically evaluated. The results demonstrate that Fe₂O₃ concentration plays an important role in modifying photon transport and the angular distribution of the emitted light. The increase in Fe₂O₃ concentration enhances the scattering characteristics of the phosphor layer and consequently alters the propagation paths of blue and yellow photons. In combination with the corresponding adjustment of YAG:Ce³⁺ concentration for the 4000 K-class target, these scattering changes influence the angular CCT distribution and ΔCCT. An appropriate Fe₂O₃ concentration can therefore contribute to improved angular color uniformity. However, excessive scattering is accompanied by a progressive reduction in luminous output, indicating that stronger scattering does not necessarily result in better overall WLED performance. The color-quality results further show that Fe₂O₃ concentration affects both CQS and CRI through changes in the spectral characteristics of the emitted light. The spectral power distributions provide additional evidence that the interaction between Fe₂O₃ scattering and YAG:Ce³⁺ phosphor emission governs the resulting optical characteristics. Therefore, the selection of Fe₂O₃ concentration should consider the balance among angular color uniformity, luminous efficiency, and color quality rather than optimizing a single optical parameter. Overall, the numerical results indicate that Fe₂O₃ is a promising scattering material for controlling the optical characteristics of pc-WLEDs. The proposed approach provides a useful basis for identifying suitable Fe₂O₃ concentrations for 4000 K-class WLED applications while highlighting the inherent trade-off between enhanced scattering and luminous efficiency. Further studies incorporating experimentally validated optical parameters and experimental measurements would be valuable for confirming the predicted performance.

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