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Optical modeling based on mean free path calculations for quantum dot phosphors applied to optoelectronic devices: comment

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Abstract: A recent publication by Shin et al. [Opt. Express **25**, A113 (2017)] contains an optical simulation model for the quantum dots (QDs) nanophosphor based on the mean free path concept. We show that their measured scattering pattern of QDs is misleading, which would result in a fatal deviation between simulated and actual values.

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References and links

1. M.-H. Shin, H.-J. Kim, and Y.-J. Kim, “Optical modeling based on mean free path calculations for quantum dot phosphors applied to optoelectronic devices,” Opt. Express **25**(4), A113–A123 (2017).
2. B. Xie, R. Hu, and X. Luo, “Quantum dots-converted light-emitting diodes packaging for lighting and display: Status and perspectives,” J. Electron. Packag. **138**(2), 020803 (2016).
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Quantum dots (QDs) nanophosphors based light-emitting devices have been attracting numerous attentions in lighting and flat panel display applications, by virtue of their high luminous efficacy and excellent color rending ability. Until now, there are few literatures referring to the accurate optical model of QDs, which severely limit the design and fabrication of QDs devices. The optical simulation model based on mean free path calculations, as introduced in [1] by Shin et al., offers an important reference for those working on this issue. While, the scattering pattern of QDs, which is one of the key parameters for predicting the behavior of incident light rays in QD film, is measured in a nonstandard way and the result is misleading.

In this short communication, we discuss the potential misinterpretation caused by the scattering pattern reported in [1].

Figure 1 shows the schematic of all the possible behaviors between the incident blue photons and the QDs. The blue photons may either be scattered by QDs (light path (3)), resulting in a change of their movement direction, or be absorbed by QDs (light path (2)), and their energy is converted into QDs emission light or transformed into heat energy [2]. Besides, some of the blue photons may even pass the QDs layer without been affected at all (light path (1)).

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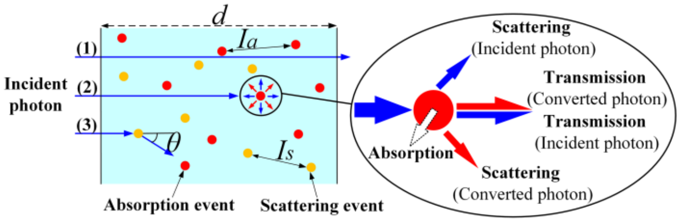

Fig. 1. Schematic showing all the possible behaviors between incident photons and the QDs-polymer film.

Accordingly, the optical properties of QDs can be characterized by three parameters, absorption coefficient μ_a, scattering coefficient μ_s, and anisotropy coefficient g [3]. The μ_s and μ_a are defined as the reciprocal of the average free path between two scattering events (I_s) or two absorption events (I_a), respectively. The g is defined as

$$g = 2\pi \int_{-1}^{1} p(v) v dv. \tag{1}$$

Where v is the cosine of the scattering angle ($v = \cos\theta$), and $p(v)$ is the single scattering phase function which characterizes the amount of light scattered at an angle θ from the incoming direction. The g ranges from −1 to 1. When $g = -1$, scattering is all directed into reverse direction, when $g = 1$, scattering is all directed into forwarding direction, and when $g = 0$, scattering is equally probable in all directions.

In the Fig. 5 of [1], the authors measured the angular distribution of the scattered light for green and red QDs with concentration of 5 wt% and 10 wt%, then this angular distribution of QDs film (or solution) was considered as the scattering pattern of QDs, and was utilized to conduct the Monte-Carlo ray tracing simulation. However, this treatment is unreasonable, since the measured angular distribution is not identical to the scattering phase function $p(v)$.Moreover, it is found that the measured angular distribution of QDs with different concentration and particle size is nearly the same, which is unreasonable from the aspect of g because the g value varies with the varying condition [3].

Therefore, we conducted a Monte-Carlo ray-tracing simulation to simulate the angular distribution measurement case in [1]. A red-emissive CdSe/ZnS QDs-polymethyl methacrylate (PMMA) polymer film with peak emission wavelength of 626 nm and thickness of 0.44 mm was utilized as the test sample. A blue laser source with a peak wavelength of 450 nm and radiometric flux of 100 mW was placed perpendicular to the sample as the excitation. The optical properties of the sample towards 450 nm blue light are $\mu_s = 1.377$ mm^{-1}, $\mu_a = 1.404$ mm^{-1}, and $g = 0.583$, measured by a double integrating sphere system [3, 4].

Figure 2 depicts the simulated angular distribution of unabsorbed (scattered plus transmitted) blue light by the QDs film sample. Our simulated results show the similar distribution with those in [1]. However, if the g value varies between −0.9 to 0.9, the simulated angular distributions nearly remain the same, i.e., no matter what the g value is, the angular distribution obtained by this measurement setup is nearly invariable.

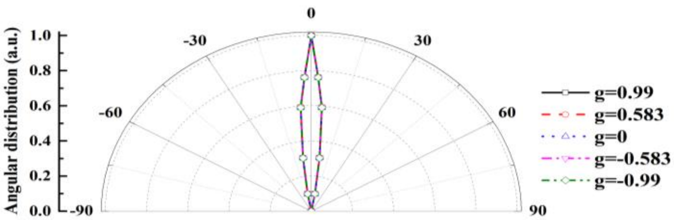

Fig. 2. Simulated angular distribution of unabsorbed blue light with varying g values.

To understand the underlying mechanism, we collected the reflected (been scattered backward), collimating transmitted (without been absorbed or scattered), and diffuse transmitted radiant flux (been scattered forward) of blue light under different g values, as shown in Fig. 3. It was found that the collimating transmitted flux changes little with the increase of g. This is predictable since the μ_s and μ_a are fixed, thus the proportion of blue light been absorbed and scattered is fixed, resulting in a fixed collimating transmittance. It was noted that the collimating transmitted flux is far larger than those of reflected and diffuse transmitted. Taking the high collimation of collimating transmitted light into consideration, the measured angular light intensity around angle $\theta = 0°$ in [1] is obviously much higher than those of other angles. Therefore, the angular distribution difference in other angles cannot be distinguished, which would introduce potential deviation. Taking $g = 0.583$ as a reference, when the g value varies between 0 to 0.9, the reflected radiant flux varies from 3.97 mW to 0.19 mW, and the transmitted radiant flux varies from 3.28 mW to 19.15 mW. Thus, the relative deviation of reflected radiant flux can reach 228% (from 1.21 mW at g = 0.583 to 3.97 mW at g = 0), and that of diffuse transmitted radiant flux can reach 87% (from 10.22 mW at g = 0.583 to 19.15 mW at g = 0.9). The large deviation will result in a fatal mismatch between the simulated and actual performances of QDs light-emitting devices [5].

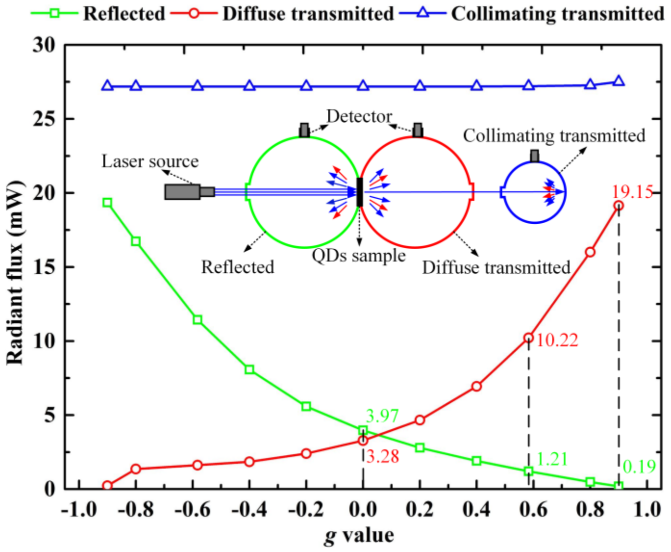

Fig. 3. Simulated reflected, diffuse transmitted, and collimating transmitted radiant flux of blue light under different g values.

Furthermore, even when excluding the collimating transmitted blue light (blue light at 0°), the scattering angular distribution of the unabsorbed blue light still remain unchanged under varying g values, as depicted in Fig. 4. Therefore, the original authors' experimental method is neither a standard nor a well-recognized approach to obtain the angular scattering distribution. At least from our result, this measurement cannot characterize the QDs scattering effect accurately.

Based on above comments, although Shin et al. provide a possible approach towards QDs optical modeling, the QDs' angular scattering properties in their model needs further corrections before it can be utilized to guide the research and development of QDs optoelectronic device.

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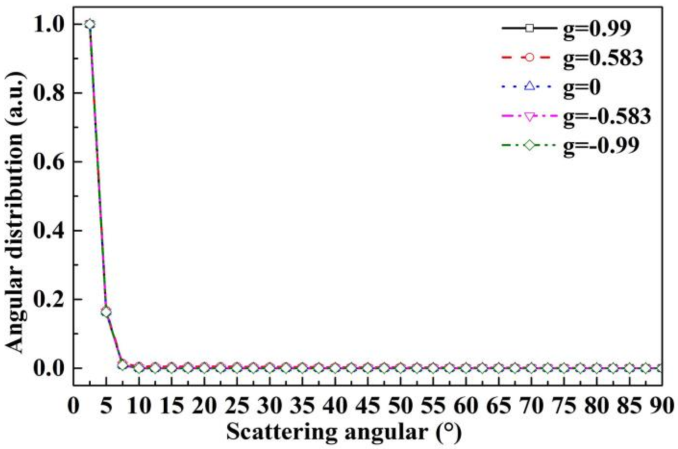

Fig. 4. Simulated angular distribution of unabsorbed blue light with varying g values when excluding the collimating transmitted blue light at 0°.

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