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Computer investigation and design of light propagation in fluorescent scattering media is considered. Suggested solution provides efficient and physically accurate model of light propagation in the media that allows simulating Stokes color shift effect and design of white LED. Based on the suggested solution the program package of simulation and design of optical devices with fluorescent scattering media was implemented and trial design of white LED was fulfilled.

Keywords: scattering media, fluorescence, fluorescence efficiency, LED, Stokes color shift, LED color design

1. Introduction

Modern, high efficient light source LED emits in very narrow spectral band often in violet-blue region that makes these LED unusable for many applications. The task of generation of white LED emission is very important and has different engineering solutions.[1)] One of possible solutions is generation of white emission as a mixture of the three primary colors (red, green, and blue) which emit colored diodes assembled in one case.[2)] Another solution is generation of white emission as a result of color shift of a fraction of the initially short-wave blue LED emission to the longer-wave spectral area.[3)] In this case output light emission which is mixture of blue and green–red spectral emissions takes white color. The color shift effect is caused by fluorescence phenomenon. There is an extensive research on phosphor-based LEDs;[4–8)] approaches used include one-dimensional light transport models (somewhat similar to the Kubelka–Munk model in paints) with account for fluorescence[7)] and two-phase ray tracing,[8)] in which we first trace light emitted from LED junction without fluorescence, obtain its spatial distribution and multiplying by phosphor "convertance" we get local source of light with shifted spectra; in the second phase this light is also traced.

We suggest a single-step ray tracing simulation, in which primary light, its conversion and propagation of the secondary light is calculated in one step. The obvious advantage is that we can cover the so-called Stokes phenomenon, when emission spectra overlaps with excitation, and thus converted light may undergo secondary conversion (that would require third pass in Ref. 8).

We use model of accurate light propagation in the materials with fluorescence properties.[9,10)] Taking into account that fluorescence material usually has finely grained structure embedded into binding material we supply our computing model with special features of light propagation in the scattering medium with micro particles (including fluorescence ones). The article presents our approach, results of simulation of color shift effect in the initially blue LED and design of white LED by means of optimal choice of concentration of scattering fluorescence particles.

2. Physical System

Fluorescence effect means that particle captures photon of one wavelength and re-emits photons of another, longer wavelength. After re-emission the photon loses polarization (i.e., becomes wholly depolarized). Angular distribution of emitted photons is assumed isotropic.

The quantitative attributes of fluorescence are: spectral density of *emission* and *efficiency* which we define as the fraction of the *absorbed* energy that is emitted; it is an integral over emitted spectrum. *Absorbed* energy, as well as without fluorescence, is due to the imaginary part of refraction index.

Light field inside micro particles is subjected to diffraction and the scattered field is described by the Mie theory (interaction of an electromagnetic wave with a sphere, see Ref. 11).

Thus fluorescence properties of a material generally depend on particle size, and differ from that of a molecular-level mixture. Light propagation in the fluorescent scattering medium can be described as a mixture of wave and ray theories of the ray propagations. While scattering by the particles has wave nature, light propagation between particles can be described by means of ray optics. This division allows utilizing model of light propagation in the scattering fluorescent medium to the light simulators based on ray tracing (Monte-Carlo solution of the light transport equation). In this case diffraction by particles is reduced to the phase function and cross sections of scattering and absorption assigned to the whole medium; ray tracer operating these cross sections and phase function only (i.e., do not know about particles).

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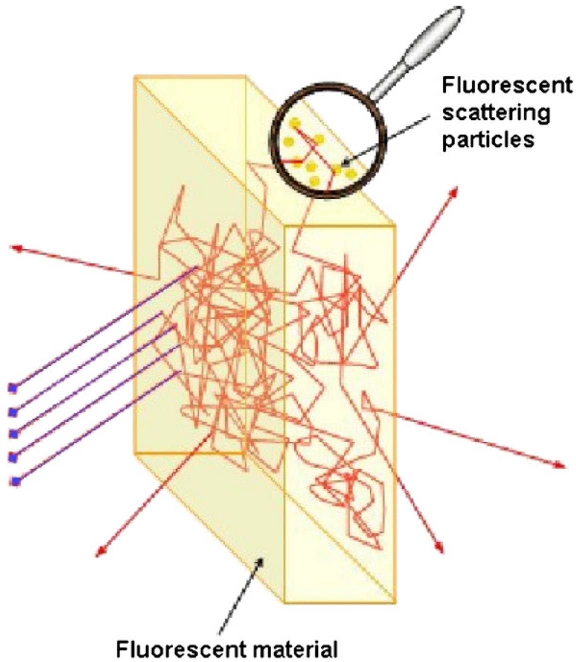


Fig. 1. (Color online) Ray propagation scheme in the material with fluorescent.

As a base of implementation of the fluorescence effect we used SPECTER software package.[12)] The SPECTER software is based on physically accurate stochastic ray tracing model and allows simulation and design of LED based devices. It allows to simulate and design both LED elements (reflectors, lenses and materials embedded to LED) and complex optical devices based on LED technologies (for example, different kinds of backlight device). So extension of SPECTER to handle fluorescent scattering phenomenon looks quite natural.

Figure 1 demonstrates and idea of the ray propagation in the material with fluorescent and scattering particles. Light photons enter to the medium with fluorescent scattering particles and are propagated in straightforward direction until scattered by particles. With probability determined by *extinction*, ray undergoes transformation. First, like for an ordinary (without fluorescence) material it can be scattered or absorbed. This scattering does not change frequency and is described by the Mie theory. If the ray is absorbed, then with some probability it is re-emitted (with another frequency) isotropically. This is fluorescence. Otherwise the ray is completely killed. The probability of re-emission of an absorbed ray is determined by so-called "efficiency" of fluorescence, and the spectrum of re-emitted ray is determined by so-called fluorescent emission spectrum.

The process of the straightforward photon propagation and scattering/re-emission is continued until the ray is either killed or leaves the fluorescent material.

3. LED Model Used in the Simulation

We investigated the example where the fluorescent cap of LED transforms originally blue emission of LED into white output light. The LED is simulated as $1 \times 1\,\mathrm{mm}^2$ area light

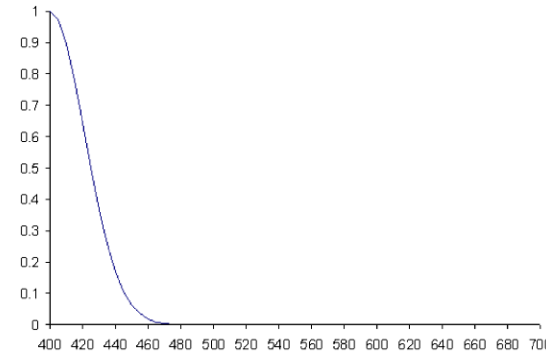
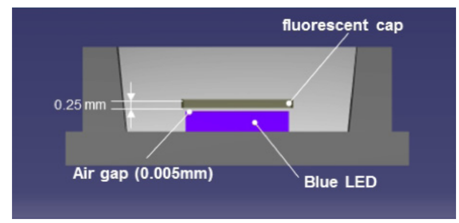
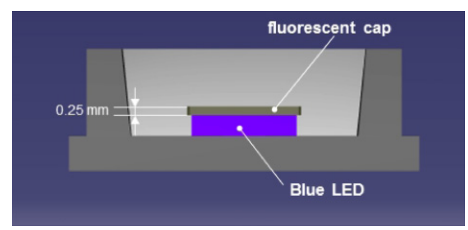


Fig. 2. (Color online) Spectrogram of LED emission.



(a)



(b)

Fig. 3. (Color online) LED geometry: (a) with air gap under fluorescent layer; (b) without air gap under fluorescent layer.

source with Lambert emission. Spectrogram of emitted light is shown in Fig. 2.

Fluorescent cap is simulated as a cylinder of height (thickness) 0.25 mm, and radius 1.25 mm, placed above the LED. Two cases of the cap placement over the LED are considered:

- There is air gap $5\,\mu\mathrm{m}$ between LED and fluorescent layer [Fig. 3(a)];
- The fluorescent layer and LED surface are in optical contact [Fig. 3(b)].

Material of the fluorescent cap consists of "passive" binder without fluorescence (refraction index 1.5) and particles of diameter $15\,\mu\mathrm{m}$ dispersed in it which are made of fluorescent substance with real part of refraction index 2.0.

In our simulation fluorescent emission and efficiency spectra were as shown in Fig. 4. It also shows imaginary part of refraction which determines absorbed energy (whose "efficiency" fraction is then re-emitted with the change of spectrum).

Our simulation covered only "optical part". Another field of interest is heat transfer and temperature distribution. In

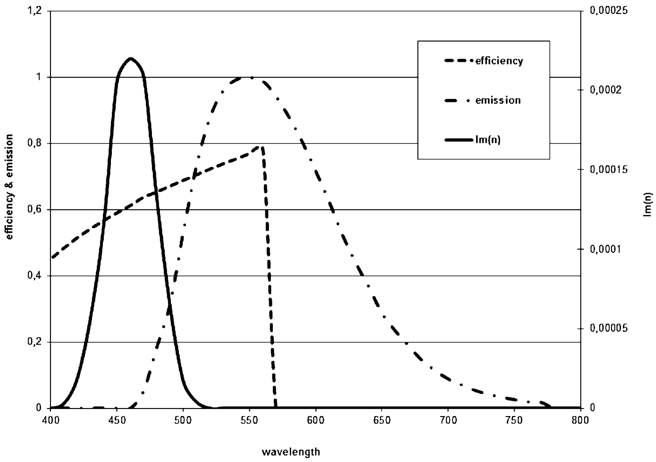


Fig. 4. Fluorescent efficiency factor of used particles for 400–480 nm.

principle, high temperature may affect phosphor properties. This can be simulated within the framework of our model. To do this, one must proceed as follows.

1. First, one performs simulation assuming some uniform temperature. Our method outputs spatial distribution of light inside LED cap. Then, multiplying by local absorption one gets the local heat dissipation, i.e., the local heat source.
2. After that, a usual heat transfer simulation is performed, see, e.g., Ref. 13. Besides heat production in the diode junction itself, we also add the above heat source due to the local light absorption.
3. Then we take non uniform phosphor properties determined by the local temperature field, input in our optical simulator and repeat simulation. Then repeat step 2, etc.

We had not any plausible measured data on phosphor dependence on temperature, so we do not present the simulation. But if the data is available one can do it with our simulation method.

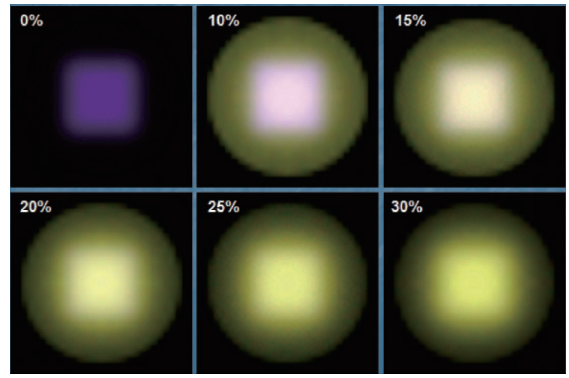
4. Results of Simulation

We performed calculations for increasing concentration of particles. When there are none of them, we see the original LED color (blue).

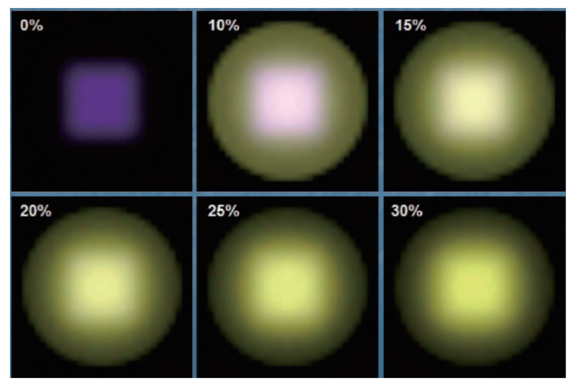
One can see that for nonzero concentration of phosphors, scattering (and fluorescence) light spreads over the whole cap, so its disk is all illuminated and visible, see Figs. 5(a) and 5(b).

In each image, Tone Mapping Operator is applied with maximal luminance taken from the brightest point (center of the image). Thus all images look about the same brightness. It is convenient to investigate the change of shade. Actually brightness decreases with concentration, though not strongly. It is the "price" of the color shift.

We present only spatial distribution of light color over the LED area. Our simulator allows to calculate angular distribution (of light emitted from a selected spot or from the whole LED) as well. But in our case the angular



(a)



(b)

Fig. 5. (Color) Luminance distribution over cap's top for different concentration of particles: (a) for variant without optical contact; (b) for variant with optical contact.

distribution was close to Lambert, did not show any nontrivial behavior and so we omit that.

Notice that for low densities light spot reproduces LED emission area while for higher densities it spreads approaching symmetric distribution because of multiple scattering (i.e., light diffusion) in the layer.

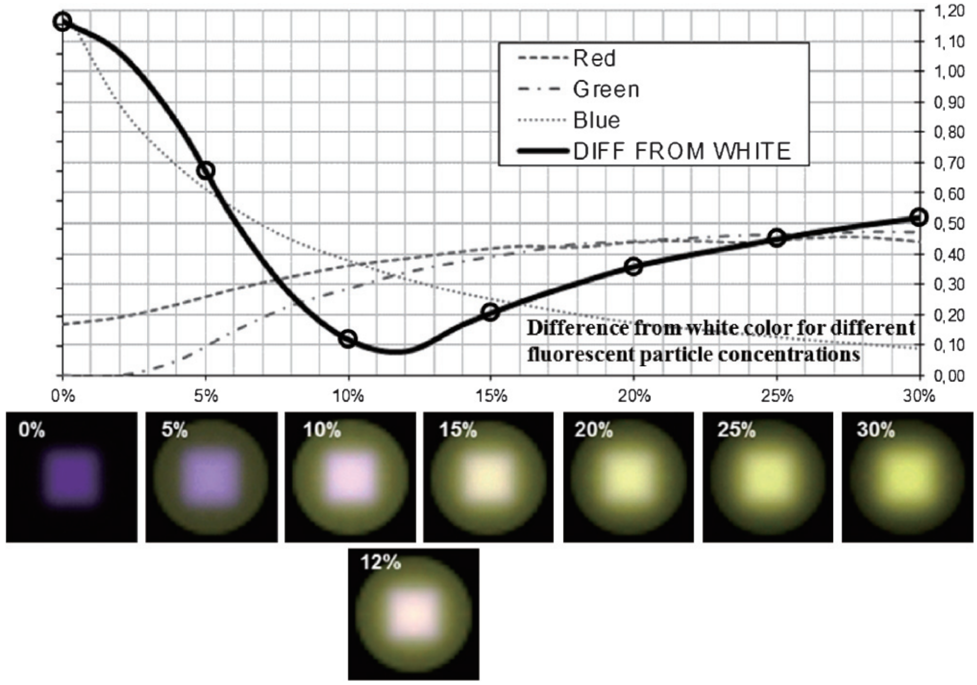
5. Design of White LED

Design aim is to achieve white color. For automatic optimization we need a quantitative criterion. A simple yet reasonable one is deviation of luminance over "central area" (above LED, see Fig. 5) from white: we take averaged R, G, B components and calculate their relative difference:

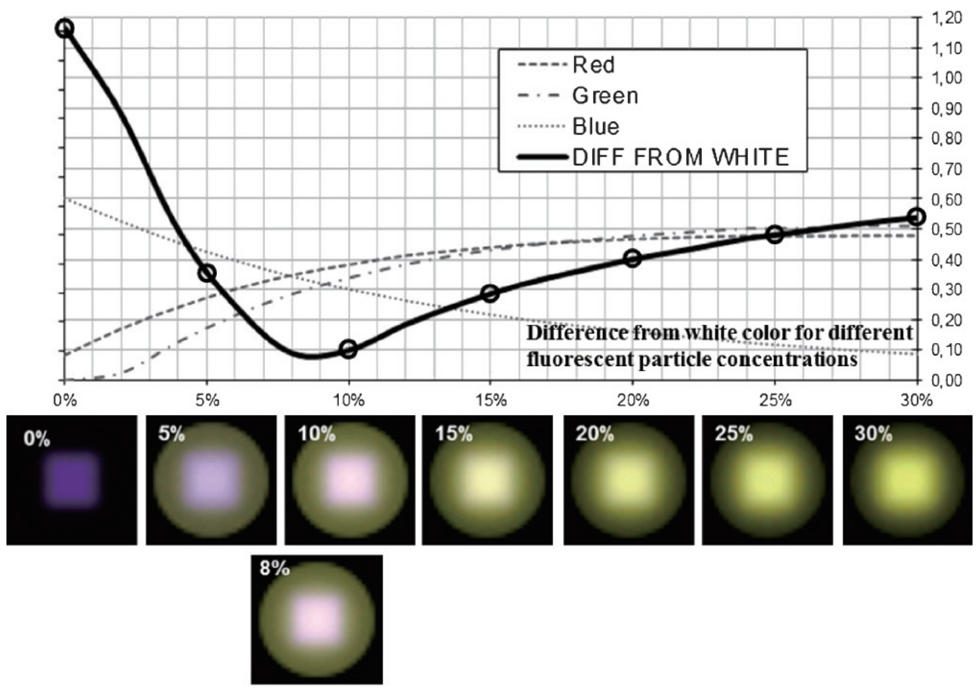
$$d = \frac{[(\mathrm{R}-\mathrm{W})^2 + (\mathrm{G}-\mathrm{W})^2 + (\mathrm{B}-\mathrm{W})^2]^{1/2}}{\mathrm{W}},$$
$$\mathrm{W} = \frac{[\mathrm{R}+\mathrm{G}+\mathrm{B}]}{3}.$$

The optimal system parameters would then minimize this d. Its plot vs phosphor concentration is shown in Fig. 6 for two variants of simulated model.

The minimum is approximately at PVC (Pigment Volume Concentration, i.e., the fraction of the whole material's volume occupied by particles) = 12% for the air gap model and at PVC = 8% for the model with optical contact. This gives the best approximation to white. Luminance values are



(a)



(b)

Fig. 6. (Color) R, G, B luminance over central area and "difference from white" d (secondary axis) as a function of concentration: (a) for the air gap model; (b) for the model with optical contact.

very high because we assigned unit flux for LED; when concentrated in the small area about $10^{-6}\,\mathrm{m}^2$ it naturally gave large luminance. Its absolute values are though irrelevant because of linearity.

6. Conclusion

The solution for a physically accurate simulation of fluorescence and volume scattering phenomena in complex optical devices like LED is elaborated. It is demonstrated that developed software is capable to design LED color. The elaborated software is embedded in the software package SPECTER.

Acknowledgment

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