A photometric investigation of ultra-efficient LEDs with high color rendering index and high luminous efficacy employing nanocrystal quantum dot luminophores

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Abstract: We report a photometric study of ultra-efficient light emitting diodes (LEDs) that exhibit superior color rendering index (CRI) and luminous efficacy of optical radiation (LER) using semiconductor quantum dot nanocrystal (NC) luminophores. Over 200 million systematically varied NC-LED designs have been simulated to understand feasible performance in terms of CRI vs. LER. We evaluated the effects of design parameters including peak emission wavelength, full-width-at-half-maximum, and relative amplitudes of each NC color component on LED performance. Warm-white LEDs with CRI >90 and LER >380 lm/W at a correlated color temperature of 3000 K are shown to be achieved using nanocrystal luminophores.

OCIS codes: (250.0250) Optoelectronics; (230.3670) Light-emitting diodes; (230.5590) Quantum-well, -wire and -dot devices; (160.2540) Fluorescent and luminescent materials; (160.4670) Optical materials; (160.4760) Optical properties.

References and links

1. S. A. Zimov, E. A. G. Schuur, and F. S. Chapin 3rd, "Climate change. Permafrost and the global carbon budget," Science **312**(5780), 1612–1613 (2006).
2. F. Scrimgeour, L. Oxley, and K. Fatai, "Reducing carbon emissions? The relative effectiveness of different types of environmental tax: The case of New Zealand," Environ. Model. Softw. **20**(11), 1439–1448 (2005).
3. S. Pacala, and R. Socolow, "Stabilization wedges: solving the climate problem for the next 50 years with current technologies," Science **305**(5686), 968–972 (2004).
4. M. H. Crawford, "LEDs for solid state lighting: Performance challenges and recent advances," IEEE J. Sel. Top. Quantum Electron. **15**(4), 1028–1040 (2009).
5. S. Nizamoglu, G. Zengin, and H. V. Demir, "Color-converting combinations of nanocrystal emitters for warm-white light generation with high color rendering index," Appl. Phys. Lett. **92**(3), 031102 (2008).
6. J. M. Phillips, M. F. Coltrin, M. H. Crawford, A. J. Fischer, M. R. Krames, R. Mueller-Mach, G. O. Mueller, Y. Ohno, L. E. S. Rohwer, J. A. Simmons, and J. Y. Tsao, "Research challenges to ultra-efficient inorganic solid-state lighting," Laser & Photon. Rev. **1**(4), 307–333 (2007).
7. A. Žukauskas, R. Vaicekauskas, F. Ivanauskas, R. Gaska, and M. S. Shur, "Optimization of white polychromatic semiconductor lamps," Appl. Phys. Lett. **80**(2), 234–236 (2002).
8. S. J. Rosenthal, "Bar-coding biomolecules with fluorescent nanocrystals," Nat. Biotechnol. **19**(7), 621–622 (2001).
9. E. F. Schubert, *Light-Emitting Diodes* (Cambridge University Press, 2006).
10. A. R. Robertson, "Computation of correlated color temperature and distribution temperature," J. Opt. Soc. Am. **58**(11), 1528–1535 (1968).

1. Introduction

Today CO_2 content in the atmosphere is increasing because of the fossil based energy production throughout the world [1]. To slow down the increase, scientists continue to search for energy saving and energy efficiency in different fields of science [2,3]. One of the related research areas is the solid state lighting, which can potentially decrease the energy consumption for lighting by fifty percent if the light emitting diode (LED) performance targets are realized [4]. To this end, since colloidal semiconductor quantum dot nanocrystals (NCs) exhibit favorable properties including tuneable emission wavelength, easy processing, and reasonable quantum efficiency, LEDs involving nanocrystal luminophores have recently attracted significant attention for high-quality white light generation [5].

The quality of a white light source is evaluated by various performance parameters. Among them, color rendering index (CRI) is the measure of color rendition of the white light source. The best color rendition is expressed with a CRI of 100, whereas the CRI of the poorest color rendition is expressed as -100. Another important performance parameter is the luminous efficacy of optical radiation (LER), which represents the optical efficiency of the light source perceived by the human eye. Furthermore, the quality of the light source is also evaluated in terms of the correlated color temperature (CCT), which illustrates the temperature of a closest Planckian black-body radiator to the operating point on the chromaticity diagram.

Warm white light sources with high CRIs and high LERs require the generation of a white emission spectrum by strategically selected colors with the lowest possible full-width-at-half-maximum (FWHM) values, as reported by Phillips *et al*. [6]. Our group previously reported that this requirement can be met in principle using semiconductor nanocrystal quantum dots. However, optical parameters including the peak emission wavelength (WL), full-width-at-half-maximum (FWHM), and the relative amplitude of each NC color component need to be carefully designed to achieve such high-quality white light generation with CRI>90, LER>380 lm/W at a warm CCT (i.e., CCT<4000 K), which can compete with conventional white light sources [6]. Nevertheless, the previous works including ours and others have not addressed these requirements of ultra-efficient performance with CRI>90 and LER>380 lm/W using NC luminophores. Additionally, the fundamental relationship and trade-offs between CRI, LER, and CCT are still not completely understood for the case of luminophores with narrow FWHMs such as NCs. To date, only the dependence of CRI and LER at 4870 K has been reported with only 2000 different spectra [7]. In this work, we present the required parameters for high-quality warm white light generation as well as the relationship and trade-offs between the performance parameters of the light source by investigating 237,109,375 designs.

2. Calculations

We developed a computational approach to evaluate different LED designs photometrically. In our simulations, the emission spectrum of NCs is modeled as a Gaussian function [8]. The chosen wavelength intervals for each color source are swept with a 10 nm step size between 450 nm and 490 nm for blue, between 500 nm and 540 nm for green, between 550 nm and 590 nm for yellow, and between 600 nm and 640 nm for red. In addition, FWHM of each color component is changed between 30 nm and 54 nm with a step size of 6 nm. Furthermore, the amplitude of each color component spectrum is varied by multiplying with an integer between 1 and 5. Subsequently, the amplitudes of every color component are normalized to 1000 for easy comparison with other spectra. By considering all of the different spectral combinations, a total of 237,109,375 possible emission spectra have been systemically generated and investigated using [9] for LER and CRI calculations and [10] for CCT computations.

3. Results

To obtain warm white light sources with CRI >80, LER >300 lm/W at 1500 K< CCT < 4000 K, the generated emission spectra are selected and tested. As a result of the simulations, only 4,896,155 spectra are left, which correspond to ca. 2% of the entire spectra generated. When the spectra with CRI<90 and LER<380 lm/W are filtered out, the number of remained spectra is decreased to 3192, corresponding to ca. 0.001% of the entire number of spectra tested. This finding shows that efficient white LEDs (WLEDs) with high color quality are in fact hard to achieve. Therefore, it is very critical to understand the effect of the input parameters on the performance criteria and also the trade-offs between them.

3.1 Input independent analysis

To understand the relationships between CRI, LER, and CCT, the graph of CRI vs. LER is presented in Fig. 1 by only considering the data satisfying 2450 K<CCT<2550 K, 2950 K<CCT<3050 K, and 3450 K<CCT<3550 K. The investigation of these graphs shows that in all of the CCT cases, CRI decreases as LER increases. This relationship makes it clear that the performance in terms of CRI should be sacrificed to obtain high optical efficiency. Additionally, it is observed that the highest possible CRI value decreases when CCT increases. However, this change is not significant so that it is still possible to obtain high-quality warm WLEDs with high CRIs at low CCTs. For example, theoretically it is possible to achieve an emission spectrum satisfying LER>380 lm/W and CRI>90 below a CCT of 2500 K (at CCT=2326 K). Another important result of the input independent analysis comes out to be the increase of the highest achievable LER when CCT increases. Thus, there is a trade-off for obtaining high efficacy and warm color temperature at the same time. Furthermore, as CCT increases, the slope of the curve gets gentler at the same LER value on the border. This shows that the change of CRI with respect to LER slows down as CCT increases.
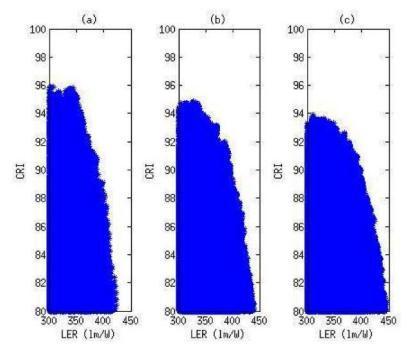

Fig. 1. CRI vs. LER dependence between (a) 2450 K<CCT<2550 K, (b) 2950 K<CCT<3050 K, and (c) 3450 K<CCT<3550 K.

The relationships of CRI vs. CCT, CRI vs. LER, and LER vs. CCT are investigated and the results are shown in Fig. 2(a), (b) and (c), respectively. In Fig. 2(a), the highest obtainable CRI value increases from 1500 to 2200 K. After 2200 K, CRI starts to decrease. The analysis of the spectra at the boundaries reveals that these points in the region between 1500 K and 2200 K have LERs approximately 300 lm/W, which is due to our restriction of LER>300 lm/W in our calculations. After 2200 K, however, the boundary LER values are much higher than 300 lm/W, and this is the region where the fundamental trade-off between CRI and CCT appears. In Fig. 2(b), the maximum obtainable CRI does not change significantly for low LER values between 300 and 330 lm/W; however, further increasing LER causes CRI to decrease. This relation between CRI and LER is expected because if one source has a high CRI, its spectrum should have a power distribution covering the visible region. Therefore, LER decreases with wider emission spectrum. Also the analysis of the boundary points shows that there does not exist a general trend between CCT and CRI. By analyzing together with the results of the previous analysis, we conclude that the border of the CRI vs. LER graph is formed by the limiting trade-off of CRI vs. LER at different CCT levels. As shown in Fig. 2(c), the increase of LER requires the increase of CCT. To obtain light sources with high LERs, the generated spectra should be cooler because the power spectral distribution around the peak of the eye sensitivity function increases. If we investigate the points with the highest LERs, these points are observed to exhibit CRI values very close to our restriction of 80, which limits the LER vs. CCT graph.
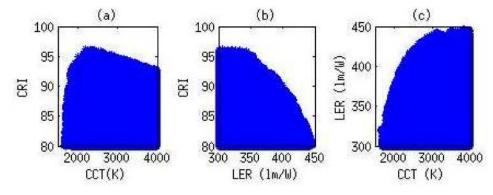

Fig. 2. Relations between **(a)** CRI and CCT, **(b)** CRI and LER, and **(c)** LER and CCT.

We further investigate whether the analyzed spectra fall in the white region on CIE 1931 chromaticity diagram. This analysis, however, requires a mathematical definition of the white region, but such a commonly accepted or widely used definition has not been found in the literature. To define the white region, we mathematically analyze the elliptic white area given in Ref. 7. By fitting this ellipse, we derive Eq. (1)-(3) to define the white region used in this work. Our analysis shows that the photometric relations for only white points (shown in red in Fig. 3) follow those for all data points including near-white points (shown in blue in Fig. 3). Noticeably, in Fig. 3 most of the data points are found to fall in the white region.

$$x' = \frac{y + 1.67x - 0.885}{1.9495} \tag{1}$$

$$y' = \frac{y - 0.607x - 0.109}{1.1648} \tag{2}$$

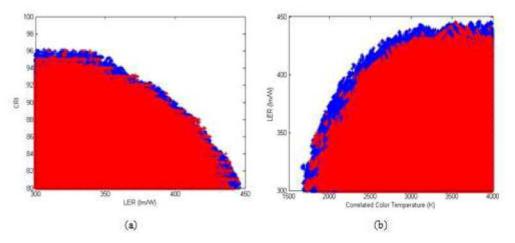$$\frac{x'^2}{0.1339^2} + \frac{y'^2}{0.0944^2} \leq 1 \tag{3}$$

Fig. 3. (a) CRI vs. LER relationship and (b) LER vs. CCT relationship for white data points (shown in red) and near-white points (shown in blue).

3.2 Input dependent analysis

The input parameters in our simulation are FWHM, relative amplitude, and peak emission wavelength. The analysis of the effects of the input parameters is carried out by calculating the average and standard deviation (stdev) of every input parameter satisfying two conditions: The first condition is CRI>80 and LER>300 lm/W and the second one is CRI>90 and LER>380 lm/W. The cases filtered using these conditions are presented in Table 1.

3.2.1 Analysis of FWHMs

When FWHM of blue, green, and yellow color components are studied for both sets of conditions, it is observed that their average is around 43 nm and their stdev is ca. 8.3 nm in both cases. Such a high stdev of FWHM and almost the same average values for both of the cases show that the choice of FWHM for these color components is not critical to obtain high performance in designing NC based WLEDs. When the same analysis is conducted for the red color region, though, significantly different results are obtained. For CRI>80 and LER>300 lm/W, the average FWHM for red is around 40 nm with a similar stdev of other color components. However, for CRI>90 and LER>380 lm/W, this average FWHM decreases to 32 nm and its stdev reduces significantly to 3.5 nm. Considering that the narrowest FWHM in these calculations is 30 nm, it can be concluded that the FWHM of the red component is very critical for high performance and the emission linewidth should be as narrow as possible.

3.2.2 Analysis of peak emission wavelengths

The comparison of both performance criteria presented above in the blue spectral region shows that the average peak wavelength of blue color remains almost the same for both cases, around 465 nm, with a relatively high stdev (12.6 and 9.1 nm). Although there is a decrease in stdev in the high performance case, it is still not a very strong restriction for high performance. This shows that blue peak emission wavelength is not so critical, as long as it is not significantly different from 465 nm.

In the green spectral region the average peak emission wavelength for both cases is ca. 527 nm, again with a relatively high stdev (11.6 and 9.1 nm). Although we observe a decrease of 2.5 nm in the standard deviation, this decreased value of the standard deviation still does not strongly restrict the choice of peak emission wavelength in green spectral range. This points out that green peak emission wavelength is not as critical either provided that it is close to 527 nm.

Table 1. Average and standard deviation values of the input parameters of the spectra satisfying the conditions of CRI>80 and LER>300 lm/W, and CRI>90 and LER>380 lm/W.

		For CRI>80 & LER > 300 lm/W		For CRI>90 & LER > 380 lm/W	
		Average	Standard Deviation	Average	Standard Deviation
FWHM (nm)	Blue	43.2	8.4	44.4	8.3
	Green	42.4	8.5	43.3	8.4
	Yellow	44.1	8.3	44.0	8.2
	Red	40.4	8.3	32.1	3.5
WL (nm)	Blue	465.7	12.6	465.1	9.1
	Green	527.0	11.6	527.9	9.1
	Yellow	574.9	13.3	569.0	9.7
	Red	625.5	9.0	620.7	2.5
Relative amplitude (/1000)	Blue	160.9	64.3	97.5	19.6
	Green	213.2	81.1	229.0	77.5
	Yellow	243.0	78.2	241.3	71.1
	Red	383.2	75.9	432.4	48.7

In the yellow spectral region, the average peak emission wavelength for CRI>80 and LER>300 lm/W is 574.8 nm with a stdev of 13.2 nm. For CRI>90 and LER>380 lm/W, the average peak emission wavelength is blue-shifted by ca. 6 nm. Although the standard deviation is not low (ca. 10 nm), it is still worth noting this shift of the average peak emission wavelength. By considering these results, it can be concluded that peak emission wavelength of yellow color should be around 570 nm for high performance, but high stdev allows a wider window for choosing the peak emission wavelength.

The average peak emission wavelength of the red color component is around 625 nm with a relatively high stdev (ca. 9 nm) in the case of CRI>80 and LER>300 lm/W. For CRI>90 and LER>380 lm/W, the average peak emission wavelength shifts to 620.7 nm together with a strong decrease in stdev down to 2.5 nm. This shows that one of the most critical components for high performance is the peak emission wavelength in the red spectral region. To obtain high performance, red emission peak wavelength needs to be close to 620 nm.

3.2.3 Analysis of relative amplitudes

In the case of CRI>80 and LER>300 lm/W, the average relative amplitude of blue component is around 161/1000. This value decreases to 97.5/1000 for CRI>90 and LER>380 lm/W case. This shows that the amount of blue color should be very small to obtain high performance. Additionally, the decrease of stdev from 64.3/1000 to 19.6/1000 indicates that the weight of the blue component should be close to the indicated average value.

The analysis of the relative amplitude values in the green spectral region shows that the average weight of the green component is 213.2/1000 in the case of CRI>80 and LER>300 lm/W. For the high performance case, this value increases to 229.0/1000. The stdev for both of the cases is relatively high (around 80/1000), which indicates that the relative amplitude of green component has a relatively large window because of its high standard deviation value.

For CRI>80 and LER>300 lm/W case, the average amplitude of the yellow component is observed to be 243.0/1000. In the high performance case, this value remains almost the same. Moreover, stdev values for both of the cases are relatively high (between 78.2/1000 and 71.1/1000, respectively). As a conclusion, in order to obtain high performance, the relative

amplitude of the yellow component should be around 240/1000 and the high standard deviation value allows covering a larger relative amplitude window.

Table 2. Exemplary results of the photometric computations. In the columns of WL, relative amplitude, and FWHM, the first numbers belong to the corresponding property of the blue spectrum. The other numbers in those columns stand for green, yellow, and red spectral content, respectively.

WL (nm)	Relative amplitude (/1000)	FWHM (nm)	LER (lm/W)	CCT (K)	CRI
460, 530, 570, 620	91, 182, 273, 455	36, 54, 54, 30	380	2600	90.7
470, 530, 570, 620	91, 273, 182, 455	54, 48, 30, 30	388	3000	91.7
450, 510, 560, 620	83, 167, 333, 417	30, 30, 42, 30	384	3200	91.0
460, 520, 560, 620	100, 200, 300, 400	36, 42, 54, 30	385	3400	90.8

In the lower performance case with CRI>80 and LER>300 lm/W, the average value of the relative amplitude of the red color is around 383/1000. In the higher performance case with CRI>90 and LER>300 lm/W, the red component gets stronger and the average value increases to 432.4/1000. In addition to this, standard deviation decreases from 75.9/1000 to 48.7/1000. When all of this information is considered, it turns out that the weight of the red component is very critical for high performance due to its low standard deviation. Thus the relative amplitude of red color should be as close as possible to 430/1000. According to the results of these calculations, some exemplary spectra and their performance are given in Table 2.

The average values of CRI>80 and LER>300 lm/W results in a spectrum with CRI=92.0, CCT=3308 K, and LER=352 lm/W, and the photon counts in blue, green, yellow, and red region are 132.2/1000 and 198.3/1000, 246.5/1000, and 423.0/1000, respectively. When the average values of the parameters in the high performance case (CRI>80 and LER>300 lm/W) are used, the resulting spectrum exhibits CRI=91.3, CCT=3041 K, and LER=386 lm/W, and the relative number of photons are 79.3/1000, 211.4/1000, 240.1/1000, and 469.3/1000 in blue, green, yellow, and red spectral regions, respectively. The relative spectral power distribution for the average values of input parameters for CRI>80 and LER>300 lm/W and for CRI>90 and LER>380 lm/W are shown in Fig. 4(a) and Fig. 4(b), respectively.
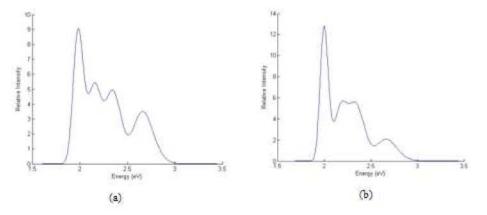

Fig. 4. The relative spectral power distribution for the average values of input parameters in the case of (a) CRI>80 and LER>300 lm/W and (b) CRI>90 and LER>380 lm/W.

4. WLED design guidelines and recommendations

To achieve WLEDs with high optical performance, it is advisable to use four colors in blue, green, yellow and red spectral ranges, as also suggested in [6]. Further recommendations can be considered in the light of Table 1, which presents a good pathway to obtain high performance. According to the results of this analysis, the color-component requirements for the corresponding peak emission wavelengths are 465.1 ± 9.1 nm for blue, 527.9 ± 9.1nm for green, 569.0 ± 9.7 nm for yellow, and 620.7 ± 2.5nm for red spectral region. Color-component FWHMs should be 44.4 ± 8.3 nm for blue emission, 43.3 ± 8.4 nm for green emission, and 44.0 ± 8.2 nm for yellow emission, considering the limitations determined by the respective standard deviation values. For the red region, however, it is important that its FWHM remains as narrow as possible (the smallest value in our simulations is 30 nm). Another significant parameter for high-quality white light generation is the relative amplitude of each color component. This should be $97.5/1000.0 \pm 19.6/1000.0$ (the weakest) for blue and $432.4/1000.0 \pm 48.7/1000.0$ (the strongest) for red, whereas the relative amplitudes of green and yellow components need to be at the medium level of $229.0/1000.0 \pm 77.5/1000.0$ and $241.3/1000.0 \pm 71.1/1000.0$, respectively.

5. Conclusion

In conclusion, the relationship and trade-offs between the performance parameters including CRI, LER and CCT of the WLEDs are presented. Additionally, the effects of the parameters (peak emission wavelength, FWHM, and relative amplitude) of each NC color component are investigated on the performance of resulting WLEDs. As a result, it is shown that the performance of ultra-efficient LEDs even with CRI>90 and LER>380 lm/W is achievable in principle using NC luminophores. If such high-quality WLEDs integrated with NCs luminophores are realized, they are expected to be used in future indoor lighting applications to provide higher quality light compared to the current light sources.

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