Modified empirical relation of spectral linewidth by incorporating doping concentration-based correction factor for GaN-based LED

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The spectral linewidth of an LED is an important parameter that varies with the semiconductor material used in its fabrication. The empirical formula for the spectral linewidth estimation of conventional LEDs exists, but it lacks the specific term that considers the device structure and doping levels in it. Hence its extension for multi-quantum well LED (MQW-LED) structures needs some correction and modification. This paper presents an empirical relation for estimating the spectral linewidth of a multi-quantum well LED based on GaN material, which considers its doping concentration. The advantage of the presented formula is that one can calculate the spectral linewidth using the semiconductor material's bandgap energy without performing any simulation or hardware implementation. The curve fitting technique has been employed for finding the correction factor in the existing empirical spectral linewidth formula. Out of many possible factors that could influence the spectral linewidth, the present work focuses on finding the effect of doping concentration in the confinement layers of the MQW-LED structure. The result can be extended to other materials and other MQW designs.

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1. Introduction

The LEDs are increasingly being used in many applications in the field of science and engineering [1]. The imagination of lighting without LED bulbs in the twenty-first century seems almost impossible [1]. To further enhance the efficiency of LED modifications in LED’s design and mathematical models has been proposed [2-5]. Some of the critical parameters associated with the LEDs are its spectral line-width and the output power level [6], [7]. The spectral line width is the most important factor determining the dispersion in many optical fiber communication systems [8]. Estimating the spectral linewidth of an LED before its fabrication is desirable, and an empirical formula has been in use in the literature [9]. To be specific, the empirical formula for estimation of the spectral line width for conventional LED is given by [9]

$$\Delta\lambda = 1.45 \times KT \times \lambda_p^2, \tag{1}$$

where $\Delta\lambda$ is the spectral linewidth in micrometers, KT is the thermal energy measured in electron volt, and λp is the peak emitted wavelength in micrometers. However, the values of the spectral linewidth $\Delta\lambda$ predicted by (1) are not in good agreement with its values obtained through measurements done with actually fabricated multi-quantum well LEDs (MQW-LEDs) or with simulation results obtained with different materials and different doping levels in a different number of quantum wells in it. For example, the spectral linewidth obtained from (1) of the LED reported in [6] is ~5.05 nm, whereas the linewidth calculated from the results of the fabricated LED is ~30 nm. Similar disagreement between the calculated spectral linewidth and actual linewidth is seen in the LED reported in [10]. Hence there is a need to modify the empirical formula given in (1) for MQW-LEDs. The modified formula consider the affect of doping concentration on the spectral linewidth. Knowing the parameter and their affect one could design the device as per the requirement of the application it save fabrication cost which is economical and the spectral linewidth as per our requirement which is effective.

The correction term can be additive or multiplicative, but in this article, a multiplicative correction factor in (1) is proposed, which considers the dependence of spectral linewidth on the doping levels in the confinement layers of the MQW-LED. The device under consideration is a GaN-based MQW LED given in [11] as the GaN is a popular choice and preferred over other available semiconductor materials in many designs of the light-emitting devices [12], [13]. The simulations are carried out in ATLAS software, and the obtained values of the spectral linewidth are fitted against doping concentrations using the curve fitting tool of MATLAB software. The spectral line width is reviewed in section 2 for the sake of completeness.

2. Review of spectral linewidth

The commonly used definition of the spectral line width of the LED is based on the full width at half maximum (FWHM) intensity in the emitted spectrum of the LED [14]. One can measure the FWHM from the curve between intensity versus wavelengths (frequency) of the emitted light from the LED. The typical curve of the emitted light intensity versus wavelength of an LED is shown in Fig. 1 reproduced from [11].

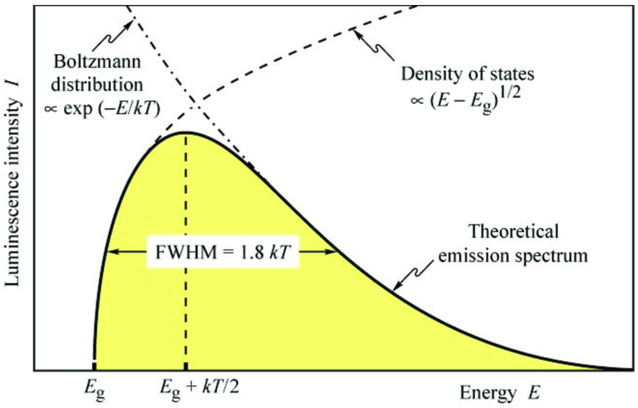

Fig. 1. Typical Emission Curve for LED [8]

The FWHM spectral width of the LED is the difference between the two wavelengths λ_1 and λ_2 where the intensity is one-half of the maximum value of the emitted light intensity and it is estimated from (1).

The estimation of the spectral linewidth ($\Delta\lambda$) of an LED is important as it determines the amount of material dispersion in the optical fiber communication system [15]. The material dispersion ($\Delta\tau$) in optical fiber is dependent on the spectral linewidth of the LED as given by the formula [16], [17]

$$\Delta\tau = \frac{L}{v_{gr}^2}\Delta v_{gr} = \frac{L}{c}\frac{d\bar{n}_{gr}}{d\lambda}\Delta\lambda \,, \qquad (2)$$

where, v_{gr} is the group velocity, L is the length of the fiber, c is the speed of light, $\bar{n}_{gr}$ is the group refractive index. From (2), it can be concluded that estimation of material dispersion in optical fiber is dependent on accurate estimation or measurement of the spectral linewidth of the LED. In the next section, spectral linewidth and its variation with doping concentration of the MQW-LEDs is analyzed.

3. Flow of proposed empirical relation

Necessity of modification: The requirement to modify the existing empirical relation of spectral linewidth (1) is arises due to asynchronization between analytical calculations and simulation results and reported linewidth in literature after actual fabrication. The spectral linewidth of LED possibly depends upon multiple parameters of the device. But the existing relation doesn't take most of the parameters into consideration while calculating the spectral linewidth. As per the existing the relation, the linewidth of all the LEDs made up of the same kind of semiconductor material should be the same, irrespective of the design, size, doping etc. which contradicts the obtained simulation results. The spectral linewidth of the device can be altered by varying various parameters of the device, it could be by changing the chemical composition, physical attributes, a combination of both chemical and physical change etc.

The following are the parameters which could impact or alter the spectral linewidth:

1. Quantum confined stark effect (QCSE).
2. Physical dimension of the device.
3. Chemical composition of combining semiconductors.
4. External doping.
5. Temperature.
6. Bandgap etc.

Out of multiple parameters, this article emphasizes on the impact of external doping on the spectral linewidth in p region of the device.

Steps followed to obtain the modified the empirical relation of linewidth.

1. (1) is rewritten in the term of bandgap energy which is more general than peak wavelength (λp).

2. The spectral linewidth of semiconductor compounds of III-V group's elements is calculated analytically by the empirical relation written in the terms of bandgap energy (4).

3. Spectral linewidth by two different method is calculated in order to check the variation. First is the spectral linewidth of an actually fabricated GaN LED reported in [6] is calculated from the EL intensity vs Wavelength curve and second is through TCAD for two different semiconductor materials GaN and InN respectively.

4. The obtained results in point 2 and point 3 are compared. As the analytically calculated results differ from the fabricated and simulated results.

5. A GaN based MQW LED is chosen and the doping concentration of p region is varied and spectral linewidth for corresponding level is recorded.

6. The relation between the spectral linewidth and doping is established by using curve fitting technique.

7. A multiplicative factor (M) obtained from curve fitting technique established the relationship between doping level and spectral linewidth.

8. M justifies the variation in results due to doping concentration.

Rules for the proposed modified empirical relation

1. Doping concentration of only P region of the LED device is varied.
2. The doping concentration covers range from $10^{20}/cm^3$ to $10^{15}/cm^3$.
3. All the physical and chemical parameters other than doping concentration remain unaltered.

Limitation and constraint of the proposed empirical relation

The modified relation is proposed and calculated by considering the GaN based LED but it might be valid to another semiconductor LED as well. In addition to in this article only the affect of doping is taken into consideration, while keeping another parameter constant. Because of this variation in spectral linewidth calculated using modified relation and actually fabricated device is most likely.

Justification of modification in the existing empirical relation of spectral linewidth

The variation in analytical calculated spectral linewidth and simulation results demands that modification is required. The variation in results is verified by simulating two different LEDs made up of different semiconductor materials.

4. Expressing empirical formula of the spectral linewidth in terms of bandgap energy

The empirical expression of the conventional LED's spectral linewidth is well-known and is given in (1). The value of photon energy E_p corresponding to the maxima emitted light intensity associated with peak wavelength λ_p (as shown in Fig. 1) is related to the bandgap energy of semiconductor material E_g and is given by [8]

$$E_p = E_g + KT/2\,, \tag{3}$$

where E_p and E_g are expressed in eV, K is Boltzmann constant, and T is the temperature in Kelvin. The amount of energy confined within the range of spectral line width is given by $\Delta E = 1.8KT$ as shown in Fig.1. For a given bandgap energy E_g of a material, E_p can be calculated from (3) and then by using the Planck-Einstein relation [18], λ_p can be obtained. Substituting the value of λ_p in (1), spectral linewidth can be obtained. However, the peak wavelength of LED is often not known before measurements are done, or simulations of the LED are carried out in software. Therefore, it is proposed here to express the relation of spectral linewidth in terms of the bandgap energy of the material. This is obtained by rewriting (1) using (3) as

$$\Delta\lambda = \frac{0.05765}{E_g^2}\,\mu m \tag{4}$$

The (4) can also be written in terms of the value of the temperature as given by,

$$\Delta\lambda = \frac{191.815T}{E_g^2}\,\mu m\,, \tag{5}$$

where T is the temperature in K and E_g is in eV.

The advantage of (4) and (5) is that one can estimate the spectral linewidth without performing any simulation or hardware realization with the prior knowledge of bandgap energy. It does not require the emitted peak wavelength E_p to determine the spectral linewidth. The problem with (5) remains the same as that with (1) in that the disagreement between calculated and simulation/actual measurement results remain as can be seen from the values of the spectral line width reported in [6] of an actually fabricated device. To illustrate this disagreement, two structures of MQW-LEDs are taken, and simulations are carried out in TCAD software, and the results are discussed in the next section.

Table 1. Spectral linewidth calculation using (5)

Semiconductor Compound	Eg (eV) at 300 K	Ep (eV) at T=300 K	λ_p (nm)	Spectral linewidth (nm)
InSb	0.17	0.18295	6.7723	1719
InAs	0.36	0.37295	3.3221	413.8
InN	0.70	0.71295	1.7378	113.2
GaAs	1.42	1.43295	0.8646	28.0
GaN	3.36	3.37295	0.3673	5.05

Using (5), the spectral linewidth of some direct bandgap semiconductor compounds of III-V group of the periodic table are calculated and are given in Table 1. These analytically calculated values from (4) will be compared with the simulated values of two semiconductor LEDs in the next section and as there is a variation in both the obtained results the modified empirical is proposed.

5. Results & discussion

In this section, to verify the difference between spectral linewidth calculated using (5) and the actual spectral linewidth of GaN and InN MQW-LEDs, simulations are carried out in the TCAD simulation tool. The spectral linewidth is calculated from emitted light intensity versus wavelength graph by calculating FWHM from the curves obtained through simulations. Thereafter the modified empirical relation is derived using curve fitting tool through MATLAB. The toolbox used in the MATLAB is the polynomial curve fitting to derive the modified empirical relation.

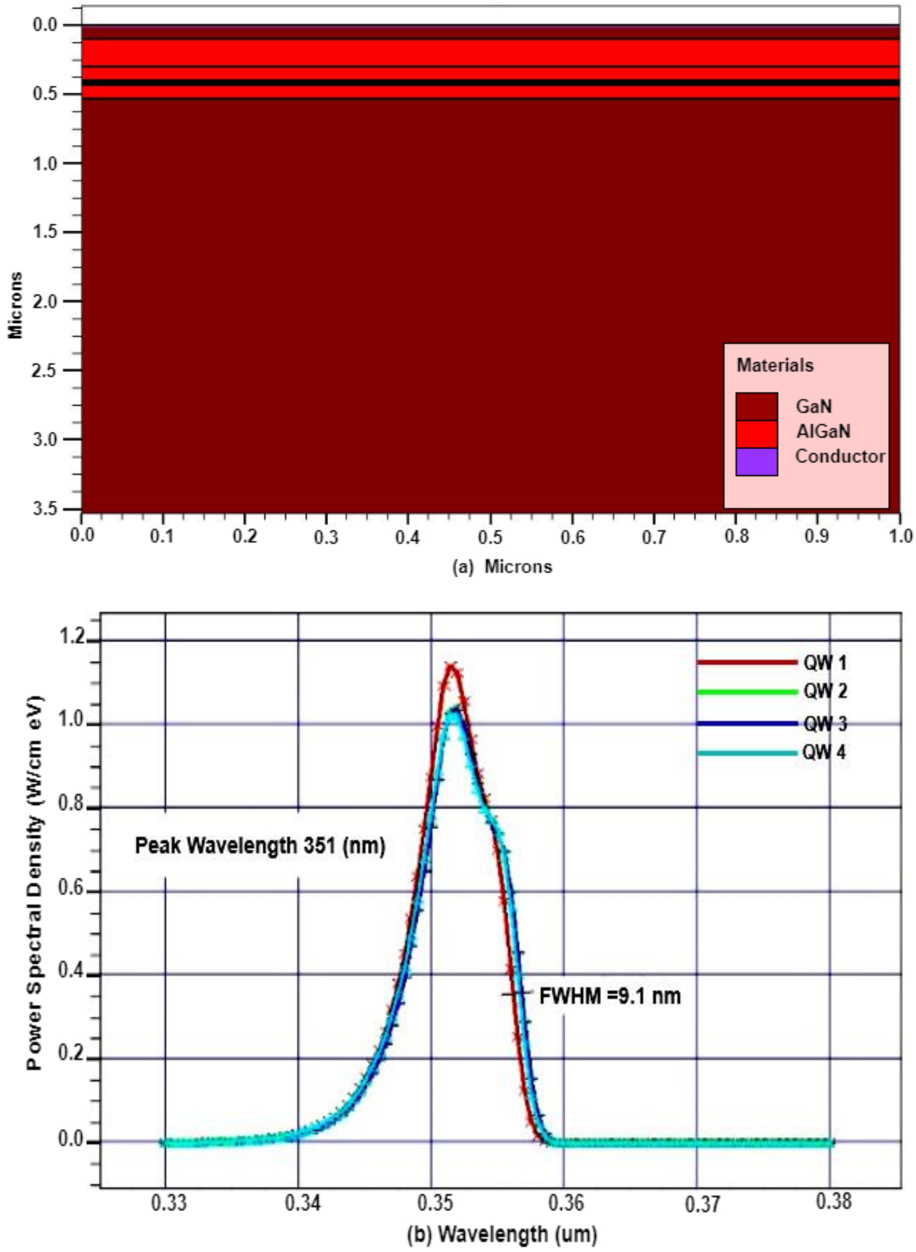

Fig. 2. (a) Simulation results of GaN MQW-LED (b) PSD vs wavelength curve (color online)

The spectral width obtained through stimulation result of the GaN-based MQW structure shown in Fig. 2 is approximately 9.1 nm. The obtained simulation results differ from analytically calculated value given in Table 1 by a considerable margin. To strengthen the claim that existing empirical relation requires modification, simulations are carried out for the structure made up of the InN LED.

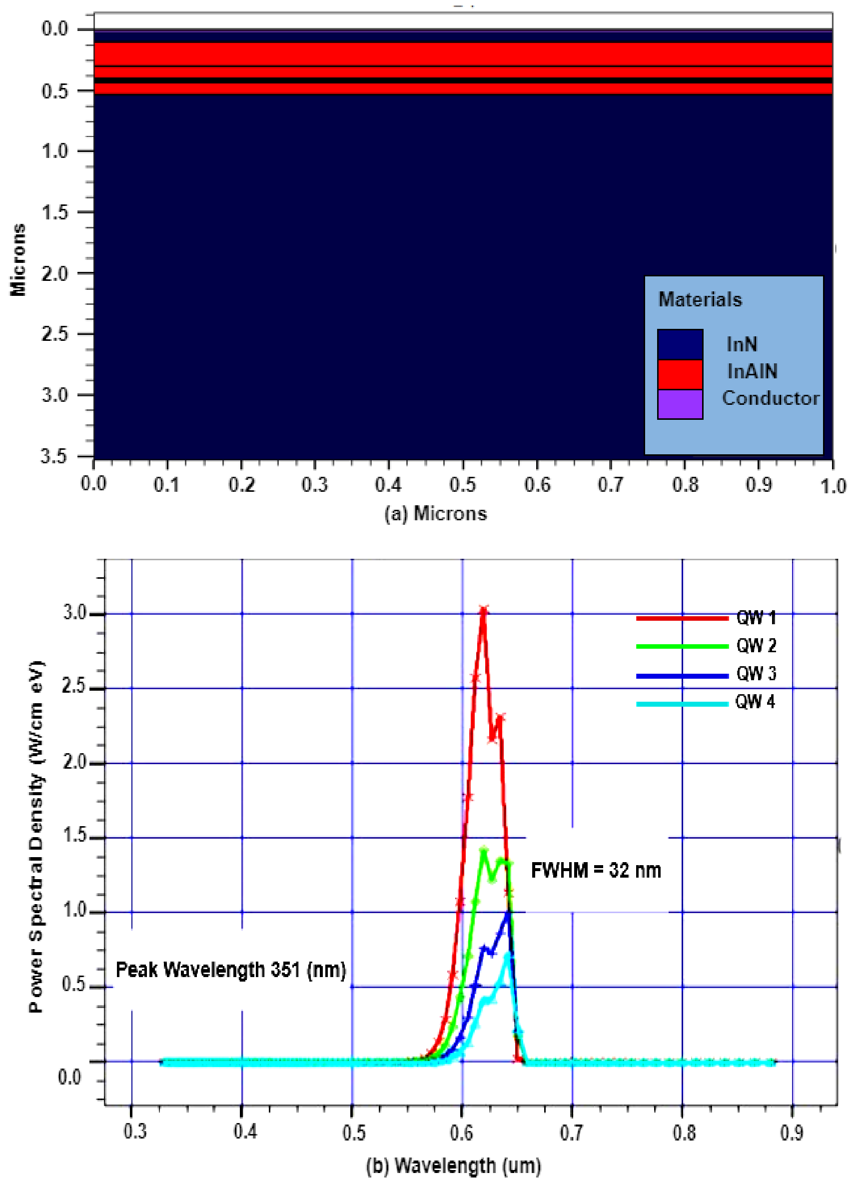

Fig. 3. (a) Simulation results of InN MQW LED (b) PSD vs wavelength curve (color online)

The InN MQW structure and the simulation results are shown in Fig. 3. The spectral line width estimated from this Fig. 3 is approximately 32 nm, which differs from the analytical value tabulated in Table 1. The difference between simulation and analytical results is possibly due to one or combination of the following reasons, external doping concentration, the mole fraction of barrier semiconductor layer, different structures (Hetero, QW, and MQW, etc.), or quantum confined stark effect (QCSE) that could influence the spectral line width. In this paper, the effects of change in the doping concentration on the spectral line width is studied.

The structure shown in Fig. 2 is used to study the effect of variation of doping concentration in the P region or the confinement layers of the MQW-LED on the spectral linewidth. The rationale behind the structure selected for study in this article is the simplicity of its shape and size and its semiconductor material. Additionally, it is a MQW structure and most of the functional LEDs in practical applications are based on MQW, and the goal of the present work is to find a suitable correction factor in the expression of spectral line width which takes into account the variation of the doping of confinement layer in a MQW structure. The selected structure design is very common and suitable to study it. In the next section the modified empirical relation of spectral line width is presented.

6. The proposed correction in the empirical formula of the spectral linewidth

The effect of doping on spectral linewidth is studied by changing the doping concentration of the P region of a

GaN-based MQW structure shown in Fig. 2. The obtained simulation results are given in Table 2.

Table 2. Doping concentration and spectral linewidth

Doping concentration ($/cm^3$) (P Region)	Simulated $\Delta\lambda$ (nm)	Analytically Calculated $\Delta\lambda$ (nm) GaN LED	Multiplicative factor (M)
10^{20}	8.67	5.05	1.735
10^{19}	8.12	5.05	1.62
10^{18}	7.71	5.05	1.54
10^{17}	7.75	5.05	1.55
10^{16}	7.77	5.05	1.55
10^{15}	7.76	5.05	1.55

The doping concentration below 10^{15}/cm^3 are not considered here as the obtained results of the emitted light intensity is very low. Within the moderate doping range, where the doping concentration is situated between (10^{15}/cm^3 to 10^{17}/cm^3) the specified limits, the influence of doping concentration on spectral linewidth is relatively minimal. This is why the rounded values presented in Table 2 are consistent. However, as the doping concentration escalates from the moderate range towards higher levels, the degree of variation becomes more pronounced. It can be seen from the results given in Table 2 differs from the computed value of Table 1. To correct this difference between results, a multiplicative correction factor *M* is proposed here.

It includes the effect of doping concentration, and is proposed as

$$\Delta\lambda = 1.45 \times KT \times \lambda_P^2 \times M \,, \tag{6}$$

where *M* is the multiplicative correction factor of order two obtained by curve fitting technique. The multiplicative factor *M* is expressed as

$$M = P_1 x^2 + P_2 x + P_3 \tag{7}$$

where P_1, P_2 and P_3 are constants and x is the doping concentration. The value of these constants is obtained through curve fitting of the data given in Table 2 and are given as

$$x = N_D \times 10^{-18}\,;$$
$$P_1 \simeq 3.445 \times 10^{21};$$
$$P_2 \simeq -1.078 \times 10^{22};$$
$$P_3 \simeq 8.427 \times 10^{21}; \tag{8}$$

The given empirical relation (6) corrects the difference between analytical and simulation-based results of the spectral line widths of the LEDs with different doping concentration in the confinement layer.

7. Conclusion

The spectral line width of an LED is an important parameter that depends on multiple factors such as structure design, semiconductor material and many more. By empirical relation (4) by merely having the prior knowledge of the semiconductor compound's bandgap energy, the spectral linewidth can be calculated. The modified empirical relation (6) includes the effect of the external doping concentration on the spectral linewidth. The proposed modified relation justifies that variation in doping could change the spectral linewidth.

8. Future scope

An integrated relation that includes all possible parameters which could affect the spectral line width remain to be studied in our future work.

References

[1] S. Rajbhandari, J. J. McKendry, J. Herrnsdorf, H. Chun, G. Faulkner, H. Haas, I. M. Watson, D. O'Brien, M. D. Dawson, Semicond. Sci. Tech. **32**, 1361 (2017).
[2] L. Sharma, R. Sharma, Opto-Electronics Review **29**(4), 141 (2021).
[3] L. Sharma, R. Sharma, Journal of Optics **49**, 397 (2020).
[4] Lokesh Sharma, Ritu Sharma, Optoelectron. Adv. Mat. **16**(7-8), 300 (2022).
[5] Lokesh Sharma, Ritu Sharma, Proc. SPIE **11995**, 1199506 (2022).
[6] A. Rashidi, M. Monavarian, A. Aragon, A. Rishinaramangalam, D. Feezell, IEEE Electron Device Letters **39**(4), 520 (2018).
[7] S. Wemple, Appl. Optics **18**, 31 (1979).
[8] E. Schubert, LED basics: Optical Properties, Light-Emitting Diodes, Cambridge: Cambridge University Press, 2nd edition, 2006.
[9] Santa Clara (CA), Silvaco International ATLAS User's Manual, Silvaco, 2018.
[10] C. Liao, Y. Chang, C. Ho, M. Wu, IEEE Electron Device Letters **34**(5), 611 (2013).
[11] A. Rashidi, M. Monavarian, A. Aragon, S. Okur, M. Nami, A. Rishinaramangalam, S. Mishkat-Ul-Masabih, D. Feezell, IEEE Photonics Technology Letters **29**(4), 381 (2017).
[12] S. N. Mohammad, A. A. Salvador, H. Morkoc, Proceedings of the IEEE **83**(10), 1306 (1995).
[13] M. Sze Simon, K. Ng Kwok, Physics of

Semiconductor Devices, Wiley-Interscience, Third Edition 2006.
[14] A. C. Carter, Radio and Electronic Engineer **51**, 341 (1981).
[15] L. D. Westbrook, M. J. Adams, IEEE Proceedings J. - Optoelectronics **134**, 209 (1987).
[16] B. Van Zeghbroeck, Principles Of Semiconductor Devices, Prentice Hall, 2006.
[17] Grant Z. Pan, Grant Z. Pan, Dae H. Pak, Jaime Peretzman, Li P. Ren, Light-Emitting Diodes: Research, Manufacturing and Applications XII, International Society for Optics and Photonics **6910**, 691015 (2008).
[18] R. Lenk, & C. Lenk, Practical Lighting Design with LEDs. (2nd. ed.) (John Wiley & Sons, Ltd., 2017).

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