Issue of spatial coherence in MQW based micro-LED simulation

Citation for the original published paper (version of record):
Wang, L., Sun, J., Yan, Q. et al (2021). Issue of spatial coherence in MQW based micro-LED simulation. Optics Express, 29(20): 31520-31526. http://dx.doi.org/10.1364/OE.438135

Research Article | Vol. 29, No. 20 / 27 Sep 2021 / Optics Express 31520

Optics EXPRESS

Issue of spatial coherence in MQW based micro-LED simulation

LE WANG,[1,2,3] JIE SUN,[2,3,4,6] QUN YAN,[2,3] JIAO LIN,[5] WEILING GUO,[1,7] ENGUO CHEN,[2,3] CHEN XU,[1] AND YONGZHEN LIU[2,3]

[1] *Key Laboratory of Optoelectronics Technology, Beijing University of Technology, Ministry of Education, Beijing 100124, China*
[2] *Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou 350100, China*
[3] *National and Local United Engineering Laboratory of Flat Panel Display Technology, College of Physics and Information Engineering, Fuzhou University, Fuzhou 350100, China*
[4] *Quantum Device Physics Laboratory, Department of Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg 41296, Sweden*
[5] *Huawei Technologies Co., Ltd., Shenzhen 518000, China*
[6] *jie.sun@fzu.edu.cn*
[7] *guoweiling@bjut.edu.cn*

Abstract: In existing flip-chip LED simulations, the light extraction efficiency is related to the multiple quantum well (MQW) to metal reflector distance because of optical interference. We calculate the contrast using several typical light intensity distributions among the several QWs in MQW. The coherence is obtained analytically. When the luminosity of each QW is equal, the contrast is ~0, meaning the light is incoherent, contrary to traditional studies. The spatial coherence is important only when the light emission comes from just one QW. As the MQW has a not negligible thickness, the traditional single-dipole model is no longer accurate.

1. Introduction

Micro-light-emitting diode (micro-LED) usually refers to an LED that is smaller than 50 µm×50 µm in mesa size. It plays a central role in the new generation of information display technology, which has higher brightness, better luminous efficiency and lower power consumption than the existing display technology. It could potentially be widely used in mobile phones, tablets, laptops, TVs, AR/VR devices, outdoor displays, head up displays (HUD) and other fields [1]. GaN-based blue micro-LED is the most important element for realizing a full color display, as the other primary colors, namely green and red, can be achieved by photoluminescence from quantum dot (QD) layer coating [2,3], although the color conversion efficiency still needs to be optimized. Clearly, it is very important to improve the external quantum efficiency (EQE) of blue micro-LEDs and push it to its limit. EQE consists of two factors, which are internal quantum efficiency (IQE) and light extraction efficiency (LEE). Recently, due to the maturity of the industrialization of GaN epitaxial wafers, the IQE can be well above 90% [4,5]. Therefore, there is not much room to greatly boost the EQE simply by improving the IQE. Hence, how to significantly improve the LEE naturally become one of the key issues for today's micro-LEDs. One of the reasons for a low LEE is because the refractive index of GaN based semiconductors is high (about 2.5), and the light outside the light extraction cone (for GaN, it is about 23 degrees [6]) is difficult to escape to the external world because of the total internal reflection (TIR). There are several ways to improve the LEE, such as adding distributed Bragg Reflector (DBR) structure, using photonic crystals, applying surface roughening technology, and implementing flip-chip technology, etc [7–9]. The flip-chip LED structure generally has a better performance than the planar and vertical structure in this regard, rendering it most suitable for micro-LEDs

#438135 https://doi.org/10.1364/OE.438135
Journal © 2021 Received 20 Jul 2021; revised 30 Aug 2021; accepted 30 Aug 2021; published 16 Sep 2021

Optics EXPRESS

[10]. Combining the above-mentioned technologies with flip-chip micro-LEDs will effectively boost the LEE.

In order to reduce the research and development cost for improving the LEE in flip-chip micro-LEDs, we often need to use simulation software to design the structure first. The main simulation methods of micro-LED are wave optics like Finite-difference time-domain (FDTD) and ray optics like Monte Carlo. The light emitting surface for flip-chip micro-LEDs is n-GaN. The p-GaN is sputtered with a layer of Ag reflector to recover the light from the back. In the wave optics based simulation, an electric dipole is used for simulating the light source, and the polarization direction of the electric dipole is parallel to the multiple quantum well (MQW) because of the special lattice structure of GaN [11]. The general simulation structure is shown in Fig. 1, where PML refers to a perfectly matched layer, PEC denotes a perfect electric conductor which is a perfect mirror, and P is the light intensity reference point. The micro-LED epitaxial structure and air constitute the whole simulation domain. A large number of earlier LED simulation studies have found that the LEE will show a strong fluctuation by changing the distance between the dipole and Ag reflector [12–14]. In fact, this effect can be very significant. For example, considering the interference between the upward and downward light beams of the electric dipole (just like two light beams in the Michelson interference experiment), when it happens to have a destructive interference and converge at the P point, the intensity of most light beams that are inside the light cone will thus be nearly 0. As the light out of the cone anyhow cannot emit to the exterior because of the TIR, the total LEE of this LED will be almost zero in this case. Indeed, this has been experimentally observed [15] and, therefore, the distance between the Ag reflector and the MQW seems to be a vital factor in LEDs and, hence, also in micro-LEDs.

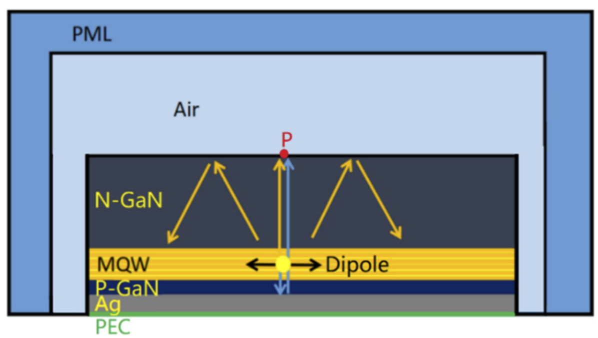

Fig. 1. Simulation diagram of micro-LEDs proposed by this study.

This notwithstanding, in this paper, we demonstrate that the optical interference induced intensity oscillation effect at changing “dipole to reflector distance” is very intense only for LEDs and micro-LEDs with single QW [15], where the experiment is consistent with the simulation. For MQW based devices, on the other hand, we have noticed that the oscillation in experiment is much weaker than the theoretically expected value [16], pointing towards a clear inconsistency between the experiments and theory. We would like to point out that there exists a misunderstanding in the community that assumes the LEE is sensitively dependent on the position of MQW with respect to the reflector in flip-chip LEDs and micro-LEDs. We think the fundamental reason for this is because the MQW has a finite thickness that can not be neglected as for the case of single QW. In optics, we know that a light source has no spatial coherence if the dimension of the source is large. That is to say, when studying the optical interference effect in today’s LEDs and micro-LEDs, the MQW simply cannot be modeled by a single dipole in the simulation. Since micro-LEDs have a much large surface to volume ratio than ordinary LEDs, the need for enhancement of the LEE appears to be even more crucial for micro-LEDs.

Optics EXPRESS

Therefore, in this work, we have analytically derived the equations on the optical coherence in flip-chip micro-LEDs and revealed that in contemporary MQW based micro-LEDs, due to the fact that the light source layers have a relatively large width, the spatial coherence is poor, and the oscillation effect mentioned above is no longer a severe concern when designing the micro-LED structures. We have considered the light intensity of each layer in the MQW with reasonable models, and calculated the contrast (defined as a variable changing from 0 to 1) at point P which is an indicator of the optical interference. We show that only when the calculated contrast is close to 1, there is a good spatial coherence, and the single-dipole model can be used to simulate the light source of micro-LEDs. Otherwise, due to the physical width of the MQW, a point light source model is no longer applicable when simulating the interference effect. Furthermore, it also weakens the effect of Purcell factor [17]. That is to say, for studying any parameters that may oscillate periodically due to the optical interference in micro-LEDs, one should seriously consider the light intensity of each layer in the MQW and calculate the contrast, instead of simply treating it as a single dipole. Although we use blue GaN micro-LEDs as an example, the physics and principles herein can also be extrapolated to flip-chip LEDs with other sizes and wavelengths.

2. Theory

Based on standard optics knowledge, the light intensity of point P in the micro-LED can be obtained from Eq. (1):

$$\mathbf{I_p} = \mathbf{I_{up}} + \mathbf{I_{down}} + 2 \times \sqrt{\mathbf{I_{up}} \times \mathbf{I_{down}}}\cos(\boldsymbol{\Delta\varphi} + \boldsymbol{\varphi}_{\mathbf{A}g}) \tag{1}$$

where I_p is the light intensity of point P, I_{up} is the upward light intensity emitted from the dipole at point P, I_{down} is the downward light intensity from the dipole which is reflected upwards to point P, and φ_{Ag} is the Ag reflector induced phase shift. Apparently, based on the electric dipole model, we have I_{up}=I_{down}. Because φ_{Ag} is constant, in order to reduce the complexity of calculation, φ_{Ag} is set to be 0. $\Delta\varphi$ is the phase shift due to the optical path difference between I_{up} and I_{down}, which in the micro-LED system can be calculated by Eq. (2):

$$\boldsymbol{\Delta\varphi} = 4\boldsymbol{\pi} \times \mathbf{D_i} \times \frac{\mathbf{N(\lambda)}}{\boldsymbol{\lambda}} \tag{2}$$

where D_i is the distance between the ith QW and the Ag reflector, λ is the vacuum wavelength, and $N(\lambda)$ is the dispersion relation of materials (the refractive index of a material is a function of wavelength [18]).

Here, just as a typical example, we assume that the MQW consists of five QWs. Thus, there are five point light sources in the device, and I is the total light intensity at point P. Plugging Eq. (2) into Eq. (1), calculating the definite integral of Eq. (1) from wavelength 400 nm to 520 nm, and making a sum of all five QWs, we have derived the total light intensity I as shown in Eq. (3), which considers the spatial coherence and temporal coherence of the MQW-based micro-LED system:

$$\mathbf{I} = \sum_{\mathbf{i}=1}^{5}\{2 \times \mathbf{QW_i} \times \int_{400}^{520}[\mathbf{I}(\boldsymbol{\lambda}) + \mathbf{I}(\lambda) \times \cos\left(4\boldsymbol{\pi} \times \mathbf{D_i} \times \frac{\mathbf{N(\lambda)}}{\lambda}\right)]\mathbf{d\lambda}\} \tag{3}$$

where QW_i is the relative intensity of the ith QW (i.e. the weight of light intensity of a specific QW among all five QWs), as shown in Table 1. When QW_i=1, it is the simplest case where all the light is emitted by the ith QW. In other cases, the total light intensity is distributed among the five QWs whose weight is characterized by QW_i (i=1, 2,. . . 5). The contrast, which is the quantitative indicator of the interference effect, is defined by Eq. (4):

$$\textbf{contrast} = \frac{\mathbf{I_{MAX} - I_{MIN}}}{\mathbf{I_{MAX} + I_{MIN}}} \tag{4}$$

Here, when the position of the entire MQW is varied by changing the thickness of p-GaN, as a result, the light intensity at point P changes. The intensity is defined as I_{MAX} when it reaches the maximum value and is defined as I_{MIN} when it reaches the minimum. The contrast can be used as a measure of the coherence. When the contrast is 1, the system is completely coherent; when the result is between 0 and 1, the system is partially coherent; when the result is 0 which means I_{max} is equal to I_{min}, the system is completely incoherent, and hence the LEE is independent of the position of MQW.

Table 1. Specific energy distribution (QW_i) of each sample

	QW_1	QW_2	QW_3	QW_4	QW_5
Sample A	0.2	0.2	0.2	0.2	0.2
Sample B	0.5	0.125	0.125	0.125	0.125
Sample C	0.8	0.15	0.05	0	0
Sample D	1	None	None	None	None

In order to improve the carrier distribution and radiative recombination rate, and reduce the electron leakage, typically, MQW with no less than five periods are manufactured in industry. In this calculation, we reasonably assume the thickness of each QW is 3 nm and each quantum barrier (QB) is 15 nm, so the thickness of the five-period MQW is 90 nm. For scientific rigor, we have assumed four different emission modes of the MQW, which are based on the literature as shown in Table 1 [18,19]. Concretely, sample A refers to the case that all the five QWs emit light uniformly which corresponds to the best situation possible for a MQW. If the MQW is not well optimized, however, QW_1 which is the nearest to the p-GaN will have the strongest light intensity because the mobility of electrons is usually higher than holes and QW_1 will then have the highest concentration of holes and electrons as compared with other QWs that are relatively far away from the p-GaN [20]. Samples B and C show the cases when the light intensity is more concentrated (with different extent) towards the close-by QWs with respect to the p-GaN. It is difficult to physically measure the light intensity of each layer of QW through actual equipment, but the radiative recombination distribution described above is a reasonable assumption that can be largely confirmed by simulation [21]. Sample D indicates the extreme case when the MQW is simplified into a single QW. The setting in sample D is also the condition used in traditional simulation, which in this paper we will prove it inappropriate for simulation for MQW based micro-LED devices.

We have measured typical blue micro-LED emission spectrum and dispersion curve as shown in Fig. 2, which are needed to calculate the temporal coherence. We assume the dominant wavelength of the micro-LED is at 458 nm, and the refractive index of the GaN-based materials in the micro-LED is 2.5 (both for the MQW and other epitaxial layers). Therefore, the corresponding wavelength in the GaN-based material is converted to about 180 nm, which is only twice the thickness of the MQW. We note that this means, according to physics, the spatial coherence will be dramatically weakened simply because the dimension of the light source is large enough as compared with the wavelength.

Optics EXPRESS

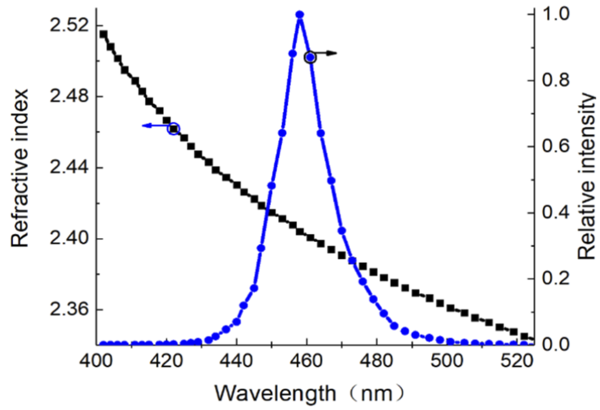

Fig. 2. Spectrum of blue micro-LEDs and dispersion relation of typical GaN-based materials.

3. Results and discussion

Using the theory and method above, we have calculated the light intensity and the contrast (see Eq. (4)) by changing the thickness of p-GaN (from 0 nm to 200 nm) in the micro-LED for four different MQW luminescence modes (labeled as samples A-D). The calculated results are shown in Table 2. According to this table, the contrast of sample D is close to 1, which means the spatial coherence and temporal coherence are very good. When the thickness of p-GaN is changed, the light intensity will oscillate strongly. This result agrees well with many earlier simulation studies, which took it for granted that there was very good spatial coherence in the device. However, this conclusion is inaccurate if we consider the MQW as several QWs with different kinds of light intensity distribution (samples A, B, C). The contrast of sample A is close to 0, which according to the discussion above means the MQW system has almost no coherence at all.

Table 2. Calculated contrast of four MQW luminescent modes of the blue micro-LED

	I_{MAX}	I_{MIN}	Contrast
Sample A	7.480	6.554	0.066
Sample B	9.451	4.585	0.347
Sample C	12.821	1.151	0.835
Sample D	14.040	0.030	0.996

The specific data for the light intensity at point P is shown in Fig. 3. Clearly, when the light emission is evenly distributed among the five QWs i.e. the case of sample A, it shows the completely opposite result as compared to the case of sample D, where the light emission is from just one single QW of the MQW. As for samples B and C, they lie between the two extreme cases. From sample B to sample C, not surprisingly, the dependence of the light intensity at point P on the thickness of p-GaN gets larger, because the light distribution is more concentrated towards one single QW, in other words more close to sample D.

With the modern development of LEDs and micro-LEDs, the uniform light intensity distribution among the individual QWs in the MQW is being aggressively pursued. Therefore, when using wave optics to design flip-chip micro-LEDs, we can no longer rely on the conventional single-dipole model to study the cavity effect. That is, a multiple-dipole model has to be applied to simulate the MQW where the light is emitted from several QWs. However, the multiple-dipole model also has an issue that needs to be practically balanced. In simulation softwares, the emissions from the several dipoles are always set to have the same initial phase, which is different

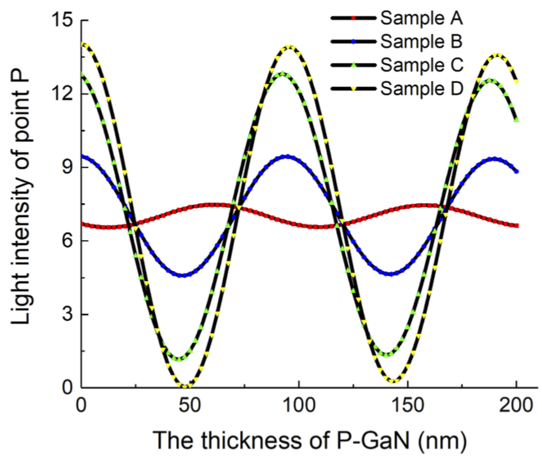

Fig. 3. The light intensity at point P of the four samples varies with the thickness of the p-GaN.

from the reality with random initial phases. In other words, in simulation the dipoles are coherent, which is an artifact. To get rid of this discrepancy, one could simulate the dipoles one at a time, and finally add them up. This is physically correct, but will take more simulation time, and is expected to be addressed by future more powerful tools.

We note that in micro-LEDs, the thickness of p-GaN also has a great influence on the antistatic ability of the device, as well as the uniformity in the current spreading. Therefore, if the emission distribution of the MQW is uniform and yet the single-dipole model were used, a wrong calculation result on the p-GaN thickness might lead to very serious problem. In that case, based on our result, the fluctuating LEE phenomenon could simply be ignored and the interference should not be considered in the design of p-GaN thickness in the incoherent system. The traditional single-dipole model is useful only for single QW LEDs or for MQW LEDs where just one individual QW is lighting (usually occurs in a non-optimal design and electron-hole recombination dominantly happens in the QW closest to the p-GaN). On the other hand, this work should not be regarded as a total negation of using wave optics to simulate flip-chip micro-LEDs, but during the simulation, we do need to consider the light output of each individual layer of the MQW.

4. Conclusion

In summary, we have used the concept of contrast to study the optical interference in flip-chip packaged micro-LEDs that are the key elements in the next generation display technology. We have proved that a single-dipole model can not well represent the MQW structure that has a finite thickness of the order of 100 nm. We have derived an analytical formula to calculate the coherence of micro-LEDs, and also calculated the contrast at point P in the device. It is found that the coherence is very poor, almost 0 when the light intensity distribution between the QWs in the MQW is uniform. Our calculation results provide an explanation why it is difficult to experimentally observe the expected intensity oscillation from traditional single- With the development of modern micro-LED technology, the light intensity of each QW tends to be the same, and the contrast will then reduce to nearly 0 which means the device is essentially an incoherent system. Using a single-dipole as the light source in the simulation will bring a misleading design on GaN based blue micro-LEDs, and this conclusion can be extended to devices with other dimensions and wavele dipole based simulation by changing the thickness of p-GaN in actual LEDs and micro-LEDs. ngths as well. Therefore, the MQW should better be modelled by several dipoles. This being said, using several electric dipoles for multiple times in wave optics based simulation may significantly increases the simulation time, especially in 3D simulations. More powerful simulation tools are badly needed in the future to address this issue.

Funding. National Key R&D Program of China (2018YFA0209000); Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China (2020ZZ110, 2021ZZ122); National Natural Science Foundation of China (62175032).

Acknowledgment. We thank the National Key R&D Program of China, the Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China and National Natural Science Foundation of China for this work.

Disclosures. The authors declare that there are no conflicts of interest.

Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

References

1. Y. Huang, G. Tan, F. Gou, M. C. Li, S. L. Lee, and T. S. Wu, "Prospects and challenges of mini-LED and micro-LED displays," J. Soc. Inf. Display **27**(7), 387–401 (2019).
2. G. S. Chen, B. Y. Wei, C. T. Lee, and H. Y. Lee, "Monolithic red/green/blue micro-LEDs with HBR and DBR structures," IEEE Photonics Technol. Lett. **30**(3), 262–265 (2018).
3. F. Gou, E. L. Hsiang, G. Tan, and P. T. Chou, "Angular color shift of micro-LED display," Opt. Express **27**(12), A746 (2019).
4. H. Y. Ryu, G. H. Ryu, Y. H. Choi, and B. Ma, "Modeling and simulation of efficiency droop in GaN-based blue light-emitting diodes incorporating the effect of reduced active volume of InGaN QWs," Current Appl. Phys. **17**(10), 1298–1302 (2017).
5. C. M. Ma, M. Tian, P. Li, J. S. Mo, W. L. Niu, T. Lin, and Z. C. Feng, "A new model on recombination dynamics of polar InGaN/ GaN MQW LED and IQE measurement," Semicond. Sci. Technol. **35**(5), 055011 (2020).
6. Z. Y. Qi, X. L. Hu, and H. Wang, "Design of surface textures for high light extraction efficiency GaN-based flip-chip TFLEDs," Chin. J. Lumin. **38**(3), 338–346 (2017).
7. C. Huh, K. S. Lee, E. J. Kang, and S. J. Park, "Improved light-output and electrical performance of InGaN-based light-emitting diode by micro roughening of the p-GaN surface," J. Appl. Phys. **93**(11), 9383–9385 (2003).
8. T. Fujii, Y. Gao, R. Sharma, E. L. Hu, S. P. DenBarrs, and S. Nakamura, "Increase in the extraction efficiency of GaN-based light-emitting diodes via surface roughening," Appl. Phys. Lett. **84**(6), 855–857 (2004).
9. J. J. Wierer, A. David, and M. M. Megens, "III-nitride photonic-crystal light-emitting diodes with high extraction efficiency," Nat. Photonics **3**(3), 163–169 (2009).
10. Y. Feng, C. B. Liu, Z. Cheng, and Z. J. Liu, "Study on flip-chip structure of GaN based micro-LED. SID Symposium Digest of Technical Papers," Dig. Tech. Pap. - Soc. Inf. Disp. Int. Symp. **51**(1), 132–135 (2020).
11. S. L. Chuang, "Optical gain of strained wurtzite GaN quantum-well lasers," IEEE J. Quantum Electron. **32**(10), 1791–1800 (1996).
12. P. Zhao and H. Zhao, "Analysis of light extraction efficiency enhancement for thin-film-flip-chip InGaN QWs light-emitting diodes with GaN micro-domes," Opt. Express **20**(S5), A765–A774 (2012).
13. H. Y. Ryu, J. Pyo, and H. Y. Ryu, "Light extraction efficiency of GaN-based micro-scale light-emitting diodes investigated using finite-difference time-domain simulation," IEEE Photonics J. **12**(2), 1–10 (2020).
14. X. M. Jin, S. Trieu, G. J. Chavoor, and G. M. Halpin, "Enhancing GaN LED efficiency through nano-gratings and standing wave analysis," Nanomaterials **8**(12), 1045 (2018).
15. Y. C. Shen, J. J. Wierer, M. R. Krames, M. J. Ludowise, M. S. Misra, F. Ahmed, A. Y. Kim, G. O. Mueller, J. C. Bhat, S. A. Stockman, and P. S. Martin, "Optical cavity effects in InGaN/GaN quantum-well-heterostructure flip-chip light-emitting diodes," Appl. Phys. Lett. **82**(14), 2221–2223 (2003).
16. C. Hums, T. Finger, T. Hempel, J. Christen, and A. Dadgar, "Fabry-Perot effects in InGaN/GaN heterostructures on Si-substrate," J. Appl. Phys. **101**(3), 033113 (2007).
17. H. Y. Ryu, "Investigation of the Purcell effect in GaN-based vertical LED structures using FDTD simulation," Opt. Quantum Electron. **48**(1), 6–9 (2016).
18. C. S. Xia, Z. M. S. Li, W Lu, Z. H. Zhang, Y. Sheng, and L. W. Cheng, "Droop improvement in blue InGaN/GaN multiple QW light-emitting diodes with indium graded last barrier," Appl. Phys. Lett. **99**(23), 233501 (2011).
19. X. T. Jia, Y. G. Zhou, B. Liu, H. Lu, Z. L. Xie, R. Zhang, and Y. D. Zheng, "A simulation study on the enhancement of the efficiency of GaN-based blue light-emitting diodes at low current density for micro-LED applications," Mater. Res. Express **6**(10), 105915 (2019).
20. T. Kawashima, H. Yoshikawa, and S. Adachi, "Optical properties of hexagonal GaN," J. Appl. Phys. **82**(7), 3528–3535 (1997).
21. P. Prajoon, M. A. Menokey, J. C. Pravin, J. Ajayan, S. Rajesh, and D. Nirmal, "Investigation of efficiency enhancement in InGaN MQW LED with compositionally step graded GaN/InAlN/GaN multi-layer barrier," Superlattices Microstruct. **116**, 71–78 (2018).