

Numerical simulation of UV LEDs with GaN and B GaN single quantum well

Asma Belaid[†] and Abdelkader Hamdoune

Department of Electrical and Electronic Engineering, Faculty of technology, Materials and Renewable Energy Research Unit, University of Abou-Bekr Belkaid, Tlemcen, Algeria

Abstract: The objective of this work is to simulate a single quantum well ultraviolet light emitting diode (LED) based on AlGa_N/Ga_N/AlGa_N and AlGa_N/B Ga_N/AlGa_N, by using TCAD Silvaco simulator. The first structure has a Ga_N quantum well taken between two layers, of n-AlGa_N and p-AlGa_N. The second one has a B Ga_N quantum well instead of Ga_N. We fix the concentration of the boron in B Ga_N to only 1% and we vary the thickness of Ga_N and B Ga_N quantum well layer from 7 to 20 nm, for the two structures. As results, we obtain respectively for Ga_N-LED and B Ga_N-LED, a maximum current of 0.52 and 0.27 mA, a maximum power spectral density of 1.935 and 6.7 W cm⁻¹ eV⁻¹, a maximum spontaneous emission of 3.34 × 10²⁸ and 3.43 × 10²⁸ s⁻¹ cm⁻³ eV⁻¹, and a maximum Light output power of 0.56 and 0.89 mW.

Key words: gallium nitride (Ga_N); aluminum gallium nitride (AlGa_N); boron gallium nitride (B Ga_N); UV light emitting diode (LED)

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1. Introduction

Group IIIA nitrides such as gallium nitride (Ga_N), and aluminum nitride (AlN) are used in many devices; they have an importance for electronic and optoelectronic applications.

Ga_N has demonstrated its superiority to achieve high ultraviolet light-emitting diodes (LEDs) performance; it admits a direct and wide band gap, great chemical and thermal stabilities^[1]. UV LEDs have attracted considerable interest due to a wide range of applications^[2-4] such as water treatment, high density optical data storage, sterilization of medical equipment, and biological imaging^[5, 6]. Each of these applications requires light sources emitting at a different UV wavelength^[6] where the electromagnetic spectrum is divided into regions based on the wavelength of the radiation, with the UV region defined as the wavelength range from 10 to 400 nm^[7]. In order to achieve the desired purpose of each application with high performance and optimal reliability such as cost-efficiency and energy-efficiency, many parameters should be controlled, for example the wavelength, the output power, the high densities and so. In this context recently various studies have been realized such as the using of the low-temperature barriers to improve strain relaxation and high performance Ga_N based LEDs where the authors success to increase the strain-relaxed mechanism of low-temperature barriers and address this problem^[8-12]. Maximum output power and external quantum efficiency were obtained by employing 222–282 nm AlGa_N and InAlGa_N-based deep UV LEDs fabricated on low threading dislocation density AlN template^[13], and different growth methods were proposed to obtain AlGa_N/AlN templates to obtain low threading dislocation density (TDD)^[12-14].

With a methodology based on stress management on underlying Ga_N-based epitaxial films, the authors demonstrated

numerically and experimentally that the optimal tensile stress can increase by over 100% in comparison to the LEDs with compressive stresses^[15]. Involving a simple high-quality AlN/AlGa_N buffer template on sapphire substrate which allows a remarkable improvement in the output power of 340 nm-band quaternary InAlGa_N-based UV-LEDs, however a maximum output power of 7.1 mW was reached and the authors found that the crystalline quality of the AlN/AlGa_N templates strongly affects the output power of UV-LEDs^[14].

These materials acquired many attention towards Solid-State lighting due to their continuous improvement in efficiency and longer life time when compared to other lighting systems including Compact Fluorescent Lamp (CFL) bulbs, filament bulbs etc^[16].

Recently, boron nitride (BN) has been introduced in electronic and optoelectronic components. Some of its properties have certain advantages such as electrical conductivity, high mechanical and electrical resistances, chemical stability, and optical transparency in a wide spectral range. It can be distinguished from other elements to give better performance for components; many alloys of the type B(Al, Ga, In)N have been recently proposed to take advantage of these properties^[17].

Boron nitride (BN) has some interests, particularly for its hexagonal (h-BN)^[18-22], rhombohedral (r-BN)^[19-22], and turbostratic (t-BN)^[20-23] structures. It can occur in several polymorphs, including cubic zinc blende (c-BN)^[21, 22, 23]. In its cubic structure^[24], (c-BN) has a band gap of 6.4 eV^[23].

Although the BN does not occur naturally in the wurtzite structure, one can combine the BN with AlN or Ga_N in order to obtain wider band intervals in this structure^[25].

The BN can serve as a natural extension of the family of III-nitrides such as Ga_N and AlGa_N^[26] with low concentration of B, to obtain B Ga_N, and BAlN alloys^[22].

2. Proposed structure and simulation model

Several works exist on the Al_xGa_{1-x}N/Ga_N LED structures

Correspondence to: A Belaid, belaidaasma@gmail.com

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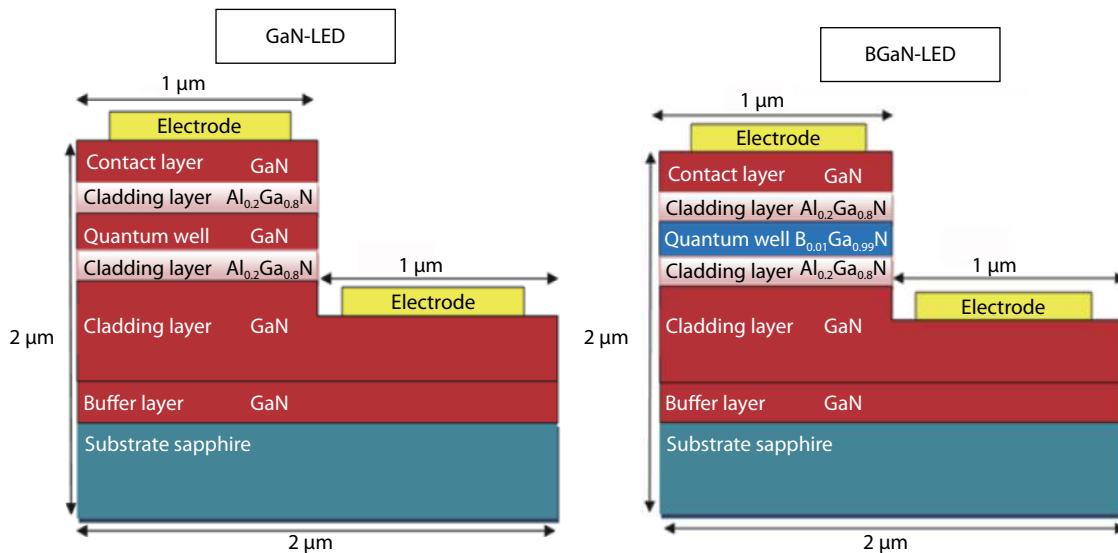


Fig. 1. (Color online) Schematic structure of UV LEDs with GaN and BGaN single quantum well.

but very little on the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{BGaN}$ LEDs. The purpose of our work is therefore to make a comparison between these two structures, using the ATLAS simulation tool. ATLAS enables device technology engineers to simulate the electrical, optical, and thermal behavior of semiconductor devices. The structures proposed with GaN and BGaN single quantum well (SQW) are shown in Fig. 1.

The GaN-LED structure consists of sapphire substrate, 5 nm GaN buffer layer, 500 nm n-doped GaN cladding layer with a concentration of $1 \times 10^{18} \text{ cm}^{-3}$, 60 nm n-doped $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ cladding layer with a concentration of $1 \times 10^{19} \text{ cm}^{-3}$, undoped GaN QW, 60 nm p-doped $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ cladding layer with a concentration of $1 \times 10^{18} \text{ cm}^{-3}$, and 120 nm p-doped GaN contact layer with a concentration of $1 \times 10^{18} \text{ cm}^{-3}$.

In the BGaN-LED, GaN QW is replaced by an undoped BGaN with a boron concentration fixed to only 1%. The band gaps of GaN, BGaN, and AlGaIn are then 3.42, 3.32, and 3.8 eV, respectively.

We consider different thicknesses for the QW: 7, 10, 15, and 20 nm.

For the binary materials (GaN, AlN, and BN), the properties are taken from the ATLAS user's manual and from references^[27, 28]. For GaN, effective density of states in the conduction band (N_c) is $1.2 \times 10^{18} \text{ cm}^{-3}$, effective density of states in the valence band (N_v) is $4.2 \times 10^{19} \text{ cm}^{-3}$, electron mobility (μ_n) is $1000 \text{ cm}^2/\text{V}\cdot\text{s}$, and hole mobility (μ_p) is $350 \text{ cm}^2/\text{V}\cdot\text{s}$.

For $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and $\text{B}_x\text{Ga}_{1-x}\text{N}$, the parameters are calculated using the Vegard law^[29]. For carrier recombination, both Shockley-Read-Hall (SRH) and Auger recombination are defined by formulas^[30, 15]; the SRH and Auger recombination coefficients are $1 \times 10^{17} \text{ s}^{-1}$ and $1 \times 10^{-34} \text{ cm}^6/\text{s}$, respectively^[15]; effective densities of states in the conduction band N_c are $3 \times 10^{18} \text{ cm}^{-3}$ and $2.35 \times 10^{18} \text{ cm}^{-3}$, respectively; effective densities of states in the valence band N_v are 1.4×10^{19} and $4.6 \times 10^{19} \text{ cm}^{-3}$, respectively. Carrier mobilities for AlGaIn are $\mu_n = 860 \text{ cm}^2/(\text{V}\cdot\text{s})$, and $\mu_p = 283 \text{ cm}^2/(\text{V}\cdot\text{s})$, respectively; for BGaN $\mu_n = 992 \text{ cm}^2/(\text{V}\cdot\text{s})$, and $\mu_p = 351 \text{ cm}^2/\text{V}\cdot\text{s}$, respectively. Saturation velocity (V_{sat}) is $2.5 \times 10^7 \text{ cm/s}$ for AlGaIn, and $2.3 \times 10^7 \text{ cm/s}$ for BGaN. The band offset between AlGaIn and BGaN is 0.48 eV and between AlGaIn and GaN is 0.38 eV.

The origin of the piezoelectric polarization is the crystal-line structure of gallium nitride. The two structures of GaN, hexagonal and cubic, are non Centro-symmetric. This mismatch between the layers induces a kind of mechanical stress, forming an interface bias charge, and thus creating what is called the piezoelectric field.

The spontaneous polarization (polarization at zero strain) is very large in wurtzite group-III nitrides resulting in a further increase of polarization induced electric fields and interface charges^[31].

A layer of gallium nitride can present a macroscopic polarization not null. There is an electric field because the crystal has an asymmetry between the barycenters of the electron charges with those of the holes. Also a link between the two atoms that is not purely covalent is a factor that can cause the creation of this electric field.

To obtain good precision, we refine the meshes in the QW layer, under the electrodes, and in the current path from the anode to the cathode.

3. Results and discussion

The Injection current versus Forward voltage is simulated for both LEDs, and for various thicknesses of the QW layer; results are illustrated by Fig. 2. In GaN-LED, the anode current decreases slightly when the QW thickness increases; the best one is of 0.52 mA (a current density of 26 kA/cm^2) for 7 nm QW thickness. In BGaN-LED, the Injection current increases more slightly with the QW thickness; the best one is of 0.27 mA (a current density of 13.5 kA/cm^2) for 20 nm QW thickness. We obtain a greater anode current in GaN-LED than that in BGaN-LED.

These results are logical because the BGaN compound is more resistive than GaN, in other words it contains fewer free electrons; in addition the charge carriers have better mobility in GaN than in BGaN.

Generation of light in LEDs is mainly due to spontaneous emission of photons, the magnitude measured by a spectrometer is the power spectral density, and the magnitude that determines the efficiency of the device is the Light output power.

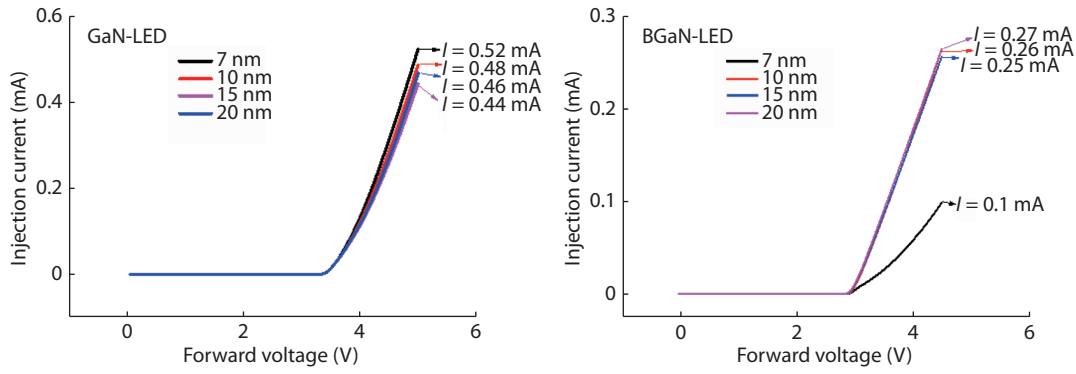


Fig. 2. (Color online) Injection current versus forward voltage for GaN-LED and BGaN-LED.

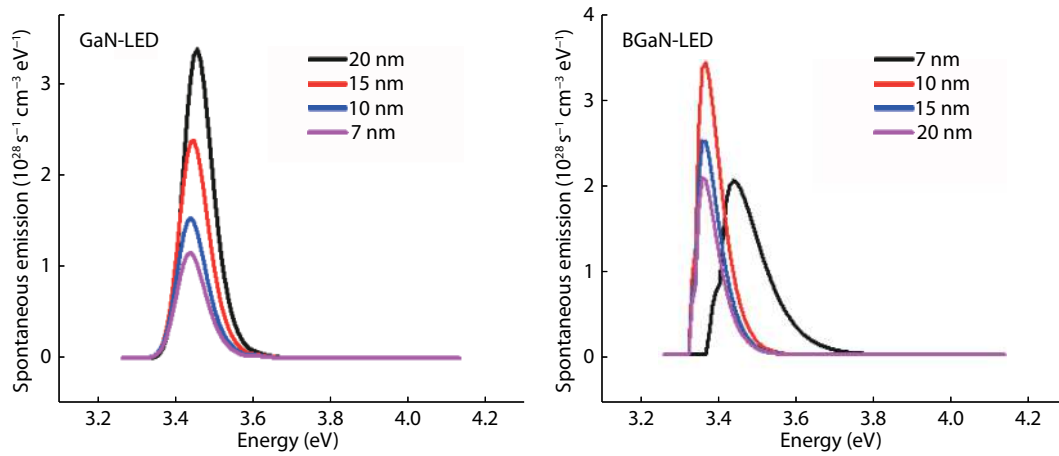


Fig. 3. (Color online) Spontaneous emission of GaN-LED and BGaN-LED.

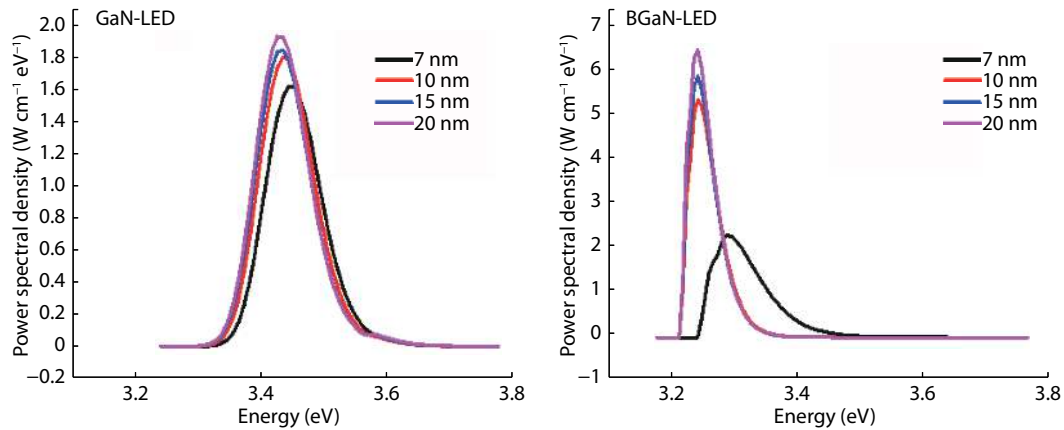


Fig. 4. (Color online) Power spectral density of GaN-LED and BGaN-LED.

Spontaneous emission, power spectral density, and light output power of GaN-LED and BGaN-LED are simulated; results are given by Figs. 3, 4, and 5, respectively. Summarized values of spontaneous emission and power spectral density are given by Tables 1 and 2, respectively.

The basic mechanisms responsible for the generation of photons in the SC are the spontaneous and the stimulated emissions.

The injected minority carriers give a light if their radiative life time is shorter than their non-radiative life time.

Band-to-band transitions can occur for example from collisions with the crystal lattice (photon-phonon interactions), or

from cascades of low energy transitions due to the presence of deep electronic levels in the forbidden band.

These deep electronic levels may be due to chemical impurities, defects in the crystal lattice (dislocations) as well as free surfaces and interfaces with other materials. The performance is limited by these nonradiative transitions.

The second and most important non-radiative recombination mechanism that limits LEDs performance is Auger recombination; it is characterized by the Auger carrier lifetimes which are inversely proportional to the square of the concentrations of the corresponding regions.

BGaN compound contains fewer free electrons; the rate of

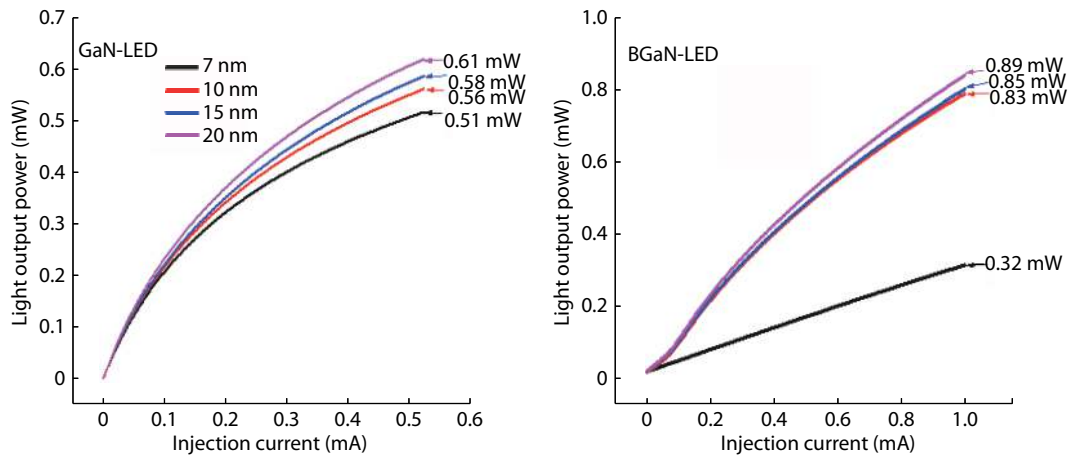


Fig. 5. (Color online) Light output power of GaN-LED and BGaN-LED.

Table 1. Summarized values of spontaneous emission for GaN-LED and BGaN-LED.

		QW thickness (nm)	7	10	15	20
GaN-LED	Peak energy (eV)		3.43	3.43	3.44	3.45
	λ (nm)		361.5	361.5	360.5	359.4
	Spontaneous emission ($10^{28} \text{ s}^{-1} \text{ cm}^{-3} \text{ eV}^{-1}$)		1.15	1.53	2.36	3.34
BGaN-LED	Peak energy (eV)		3.43	3.36	3.36	3.36
	λ (nm)		361.5	369	369	369
	Spontaneous emission ($10^{28} \text{ s}^{-1} \text{ cm}^{-3} \text{ eV}^{-1}$)		2.04	3.43	2.53	2.08
Ratio of spontaneous emissions			1.77	2.24	1.07	0.62
Difference between spontaneous emissions ($10^{28} \text{ s}^{-1} \text{ cm}^{-3} \text{ eV}^{-1}$)			0.89	1.9	0.17	-1.26

Table 2. Summarized values of power spectral density for GaN-LED and BGaN-LED.

		QW thickness (nm)	7	10	15	20
GaN-LED	Peak energy (eV)		3.46	3.45	3.45	3.45
	λ (nm)		358.4	359.4	359.4	359.4
	Power spectral density ($\text{W cm}^{-1} \text{ eV}^{-1}$)		1.61	1.81	1.84	1.93
BGaN-LED	Peak energy (eV)		3.35	3.31	3.31	3.31
	λ (nm)		370.1	374.6	374.6	374.6
	Power spectral density ($\text{W cm}^{-1} \text{ eV}^{-1}$)		2.4	5.6	6.1	6.7
Ratio of power spectral densities			1.49	3.09	3.31	3.47
Difference between power spectral densities ($\text{W cm}^{-1} \text{ eV}^{-1}$)			0.79	3.79	4.26	4.77

Auger recombination is therefore smaller in BGaN than in GaN. Thereby, in the case of BGaN, we have better spontaneous emission, better power spectral density and better Light output power.

The better value of the spontaneous emission is of $3.34 \times 10^{28} \text{ s}^{-1} \text{ cm}^{-3} \text{ eV}^{-1}$, for 20 nm of QW thickness in GaN-LED. It is of $3.43 \times 10^{28} \text{ s}^{-1} \text{ cm}^{-3} \text{ eV}^{-1}$, for 10 nm of QW thickness in BGaN-LED; and it decreases for a greater thickness because the material becomes too resistant.

The better value of the power spectral density in GaN-LED and BGaN-LED is obtained for 20 nm of QW thickness; it is respectively of 1.93 and $6.7 \text{ W cm}^{-1} \text{ eV}^{-1}$. We obtain a ratio of 3.47 between the values.

The Light output power increases with the QW thickness; better values are obtained for 20 nm of QW thickness. In GaN-LED, we have 0.61 mW at an injection current of 0.55 nA; and in BGaN-LED, we have 0.89 mW at only 0.1 nA of injection current. For this last current, the Light output power in GaN-LED is only of about 0.25 mW. We can say that the total luminous power is multiplied by 3.56 in the BGaN-LED.

There is a slight difference between the emission wavelengths in both LEDs, but the performance is significantly improved in the second LED, due to the BGaN material properties.

The flux spectral density is represented by Fig. 6, and obtained values are given by Table 3. For GaN-LED, the smallest value is obtained for the quantum well thickness of 7 nm; it is about $2.91 \times 10^{18} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$ for peak energy of 3.47 eV. For 10 nm we have a peak energy of 3.46 eV; for 15 and 20 nm, we have practically the same peak energy of 3.45 eV. For BGaN-LED, we obtain a peak energy of 3.47 eV for the quantum well thickness of 7 nm, and 3.31 eV for other QW thicknesses. The flux spectral density is, respectively, 3.25×10^{18} , 3.32×10^{18} , $3.5 \times 10^{18} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$ for GaN-LED; and 4.48×10^{18} , 1.03×10^{19} , 1.13×10^{19} , and $1.25 \times 10^{19} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$ for BGaN-LED. The peak of the flux spectral density increases with the QW thickness.

Gain TE (TE: transverse electric field), and external quantum efficiency are represented by Figs. 7 and 8, respectively.

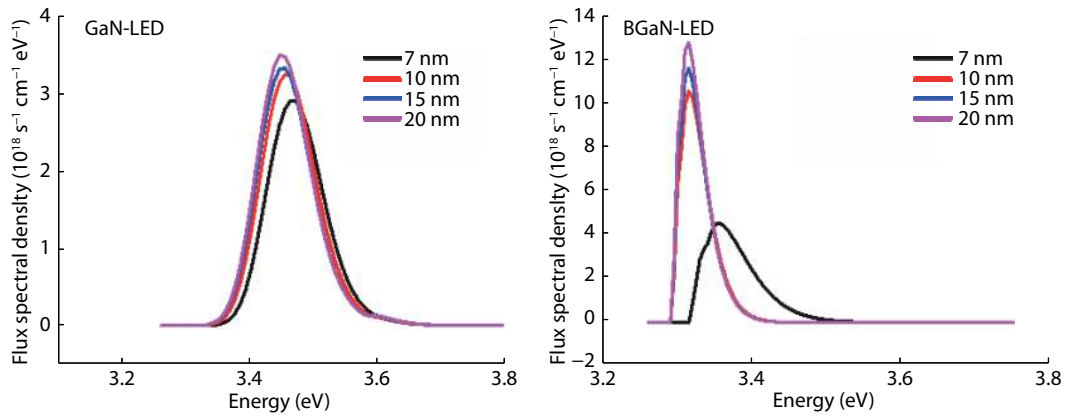


Fig. 6. (Color online) Flux spectral density for GaN-LED and BGaN-LED.

Table 3. Summarized values of flux spectral density for GaN-LED and BGaN-LED.

		QW thickness (nm)	7	10	15	20
GaN-LED	Peak energy (eV)		3.47	3.46	3.45	3.45
	λ (nm)		357.3	358.4	359.4	359.4
	Flux spectral density ($10^{18} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$)		2.91	3.25	3.32	3.5
BGaN-LED	Peak energy (eV)		3.35	3.31	3.31	3.31
	λ (nm)		370.1	374.6	374.6	374.6
	Flux spectral density ($10^{18} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$)		4.48	10.3	11.3	12.5
Ratio of flux spectral densities ($\text{s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$)			1.54	3.17	3.40	3.57
Difference between flux spectral densities ($10^{18} \text{ s}^{-1} \text{ cm}^{-1} \text{ eV}^{-1}$)			1.57	7.05	7.98	9

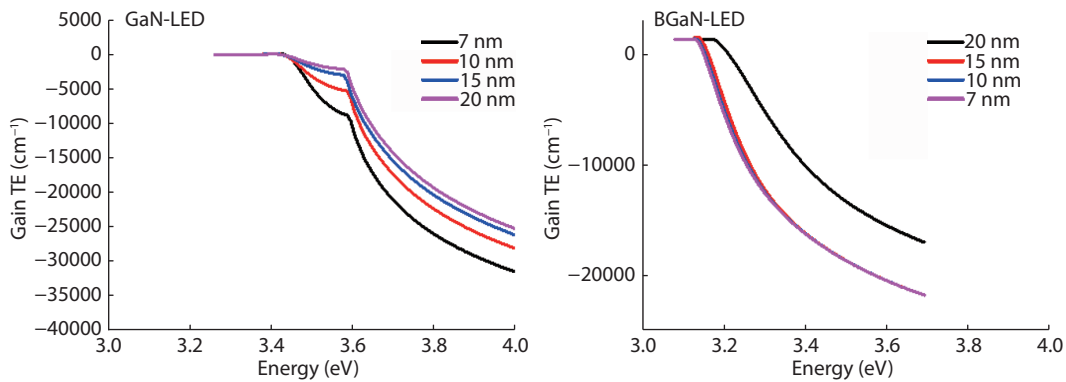


Fig. 7. (Color online) Gain TE for GaN-LED and BGaN-LED.

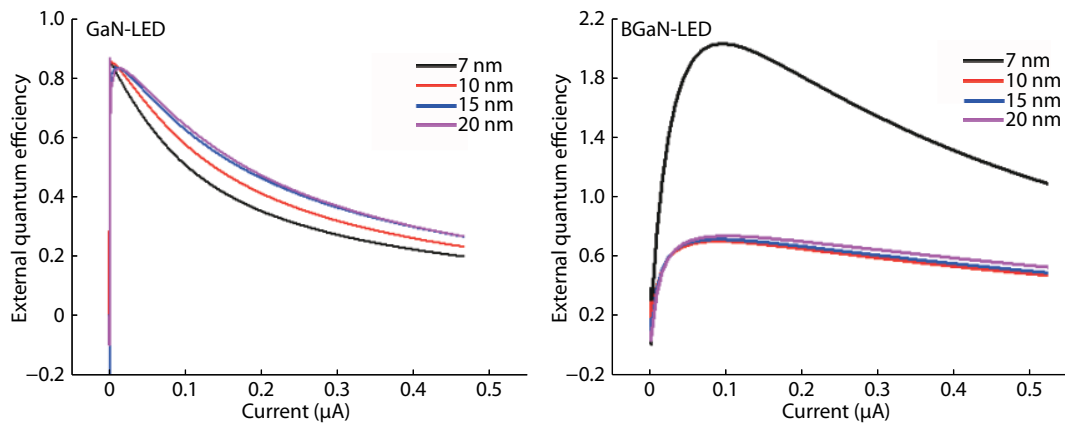


Fig. 8. (Color online) External quantum efficiency for GaN-LED and BGaN-LED.

For GaN-LED, the gain begins to decrease slowly from the energy 3.43 eV ($\lambda = 361.5$ nm), then it decreases more rapidly

from the energy 3.58 eV ($\lambda = 346.3$ nm). For BGaN-LED, the gain begins to decrease from the energy of about 3.34 eV

($\sim \lambda = 371$ nm). With BGaN, we have a slightly higher frequency bandwidth than with GaN as a quantum well.

The maximum external quantum efficiency exceeds 80% for a current of about $13.7 \mu\text{A}$ in GaN-LED, and it is of about 68% for a current of about $81.7 \mu\text{A}$ in BGaN-LED. For this second LED, we achieved a value above 100%, something we do not understand.

At a current of $0.4 \mu\text{A}$, we obtain external quantum efficiency greater than 50% for the thicknesses of 15 and 20 nm in BGaN-LED, and only 50% in GaN-LED.

4. Conclusion

AlGaIn/GaN/AlGaIn and AlGaIn/BGaN/AlGaIn UV LEDs with SQW were simulated, using TCAD Silvaco software. The boron concentration in BGaN was only 1%, and the thickness of the SQW was varied from 7 to 20 nm. In BGaN-LED; the spontaneous emission was multiplied by 1.77 for 7 nm of QW thickness, and the power spectral density was multiplied by 3.47 for 20 nm of QW thickness. The total Light output power, the frequency bandwidth, and the external quantum efficiency, were significantly improved with BGaN in the quantum well.

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