Numerical model and procedure for spectral analysis of light-emitting diode with patterned electrode

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Abstract. Two-step decomposition procedure was developed and implemented to analyze experimentally measured electroluminescence (EL) spectra of light-emitting diode with two sets of InGaN/GaN quantum wells (QWs) for blue and green emission and mesh-like top electrode. At a first step EL-spectra were decomposed into basic Gaussian functions (GFs) for blue and green emission lines. Then each of the basic GFs was decomposed into the set of secondary GFs which give reasonable ground to relate broadening of EL-spectrum to position-dependent compensation of quantum-confined Stark effect (QCSE) in the InGaN/GaN QWs. Using basic GFs it was demonstrated how injected current is splitted between green and blue QWs depending on its value.

1. Introduction

White phosphor-free monolithic light-emitting diodes (LEDs) are considered as a substitution for available white nitride-based LEDs with phosphor converters. One of the promising structures is a vertical stack of InGaN/GaN-quantum wells (QWs) with different indium concentration for emission at blue-green-red wavelengths [1, 2]. In general the electroluminescence (EL) spectra of dual-and triple-wavelength InGaN/GaN LEDs demonstrated distinctive narrow blue and green or blue, green and red (or yellow) emission lines usually with different peak intensities, separated by deep troughs [3, 4]. Growth of InGaN/GaN-QWs with high indium concentration for yellow and red light emission as well as an increase in red emission efficiency are still technological problems. Meanwhile, LEDs based on two sets of InGaN/GaN-QWs for blue and green emission and top metal electrode patterned as a mesh revealed spectra with equal peak intensities of blue and green emission lines and shallow trough between them [5]. Patterned top metal electrode has been proposed to enhance output optical performance of the blue LED [6]. Observed broad spectra of the dual-wavelength LEDs with light extraction via top surface can be attributed to the effect of meshed electrode resulting in spatially nonuniform distributions of electric potential and injected current along the QW-plane which, in turn, leads to spatially non-uniform compensation of quantum-confined Stark effect (QCSE). The latter manifests itself as spatially-dependent EL blue-shift.

In this paper, we develop decomposition procedure and implement it to analyze experimental EL-spectra of InGaN/GaN LEDs with two sets of QWs for blue and green emission and mesh-like patterned electrode.
2. Decomposition of Measured EL-spectrum

2.1. Formulation

Our analysis is based on decomposition of experimental EL-spectrum into a set of Gaussian functions. First, discretization of experimental EL-spectrum results in a set of sampling points \((\lambda_j, g_j)\), where \(\lambda_j\) and \(g_j\) are the wavelength and optical power at \(j\)-th sampling point, respectively. Then we assume that the experimental EL-spectrum can be approximated by a sum of \(N\) Gaussian functions

\[
S(\lambda) = \sum_{i=1}^{N} G_i(\lambda_i)
\]  

where \(i\)\-th Gaussian function \(G_i\) can be written in the following form:

\[
G_i(\lambda) = a_i \exp \left[ \frac{(\lambda - b_i)}{c_i} \right]^2.
\]  

Here \(a_i, b_i,\) and \(c_i\) are amplitude, wavelength at maximum and full width at half maximum (FWHM), respectively. Thus the spectrum decomposition problem is reduced to finding the coefficients \(a_i, b_i,\) and \(c_i\) for all \(N\) Gaussian functions. Total squared residual for a given number of sampling points \(M\) can be written down in the following form

\[
\Phi = \frac{1}{2} \sum_{j=1}^{M} [S(\lambda_j) - g_j]^2.
\]  

To minimize the residual (3) one needs to solve the following system of nonlinear equations for the coefficients:

\[
\frac{\partial \Phi}{\partial a_1} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial a_k} = 0,
\]

\[
\frac{\partial \Phi}{\partial b_k} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial b_k} = 0,
\]

\[
\frac{\partial \Phi}{\partial c_k} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial c_k} = 0.
\]  

2.2. Solution Procedure for System of Nonlinear Equations

The system of nonlinear equations (4) can be rewritten in the following form.

\[
\frac{\partial \Phi}{\partial a_1} = f_1(a) = 0,
\]

\[
\frac{\partial \Phi}{\partial b_k} = f_2(a) = 0,
\]

\[
\frac{\partial \Phi}{\partial c_1} = f_3(a) = 0,
\]

\[
\vdots
\]

\[
\frac{\partial \Phi}{\partial a_N} = f_{3N-2}(a) = 0,
\]

\[
\frac{\partial \Phi}{\partial b_N} = f_{3N-1}(a) = 0,
\]

\[
\frac{\partial \Phi}{\partial c_N} = f_{3N}(a) = 0,
\]  

where \(a = \{a_1, b_1, c_1, \cdots, a_N, b_N, c_N\}\), \(f_{3k-2} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial a_k}\), \(f_{3k-1} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial b_k}\), and \(f_{3k} = \sum_{j=1}^{M} [S(\lambda_j) - g_j] \frac{\partial G_k(\lambda)}{\partial c_k}\). To solve the system of nonlinear
equations (5) we apply the Levenberg-Marquardt method [7, 8]. An iterative procedure of the Levenberg-Marquardt method can be presented as follows:

\[ a^{(n+1)} = a^{(n)} + \Delta a^{(n)} \]  (6)

\[ (A + \mu I) \Delta a^{(n)} = F, \]  (7)

where matrix \( A \) and vector \( F \) comprise second and first order derivatives of (3) with respect to the unknown coefficients. Coefficient \( \mu \) in (7) should be adjusted during iterations to ensure that the coefficient matrix in the left hand side of the equation (7) is invertible.

For a given set of sampling points our spectrum decomposition procedure can be summarized as follows.

(i) Choose a set of initial values of the coefficients. Number of Gaussian functions \( N \) corresponds to the number of peaks in the spectrum under decomposition, amplitude of each peak can be used as \( a_i \), abscissa of the peak is \( b_i \), and an approximate width of the peak as \( c_i \). Number of Gaussian functions can be larger than the number of peaks.

(ii) Using equations (6) and (7), perform iterations until the length of \( \Delta a^{(n)} \) becomes sufficiently small.

(iii) During iterations, eliminate a Gaussian function if any of its coefficients reaches an unreasonable value, e.g. \( a_i \leq 0, b_i \) is beyond the range of sampling wavelengths, \( c_i \) becomes unrealistically narrow or wide. This arrangement of the algorithm allows us to use relatively rough estimate for initial guess of coefficients.

Relevant flow chart is presented in Fig. 1.

**Figure 1.** A flow chart of our spectrum decomposition procedure.

### 3. Numerical results

The proposed decomposition procedure has been applied to decompose experimentally measured EL-spectra of the LED with two sets of QWs for blue and green emission and top electrode patterned as a mesh [5]. For the EL-spectrum measured at 67 mA we set initial values for the solution \( N = 3 \), \( \{a_1, b_1, c_1\} = \{0.2, 400, 10\} \), \( \{a_2, b_2, c_2\} = \{1.3, 450, 20\} \), and \( \{a_3, b_3, c_3\} = \{1.3, 510, 20\} \) Results of decomposition into three GFs are shown in Fig. 2.
Obtained “basic” GFs have following parameters: \( \{a_1, b_1, c_1\} = \{0.26, 404.7, 15.3\} \), \( \{a_2, b_2, c_2\} = \{1.102, 451.3, 23.47\} \), and \( \{a_3, b_3, c_3\} = \{1.335, 507.3, 40.65\} \), and total residual 0.147. Basic GFs representing blue and green emission lines have FWHM equal to 23.5 and 40.7 nm, respectively, i.e., sufficiently larger than 2kT expected for thermally broadened emission [9, 10].

The third GF corresponding to a short wavelength range will be neglected in our consideration. The effect of quantum well width fluctuations and so-called alloy exiton broadening on emission line broadening was estimated as rather weak while a strain-induced piezoelectric effect (PZ) was named as much more significant contributor [9]. We believe that spatial nonuniformity of electric potential due to specific electrode configuration may contribute significantly to line broadening.

We believe that spatial nonuniformity of electric potential due to specific electrode configuration may play an important role in line broadening. To support this assumption we decompose basic blue and green GFs obtained at the previous step keeping in mind the line width due to thermally broadened emission. Results of decomposition of basic blue and green GFs into 13 and 20 GFs are shown in Figs. 3 and 4, respectively. It should be pointed out that 9 of 13 GFs for blue line and 14 of 20 GFs for green line have FWHM less than 7 nm which is quite close to that determined by thermal broadening.

Due to periodic configuration of mesh-like electrode the distributions of electric potential and injected current along the QW-active region are also periodical and spatially nonuniform within the limits of a single mesh cell. Spatial nonuniformity of injected charge carriers along the QW-plane results in spatially nonuniform screening of piezoelectric field in the InGaN/GaN QWs which, in turn, causes position dependent variations of the band gap width and emission blue-
shift, i.e., position-dependent compensation of QCSE takes place. The intensity of generated light as well as the emission blue-shift are the largest beneath the metal electrode strips and decrease to the center of the mesh opening. However, only part of the light generated beneath the strips is extracted [11, 12, 13] which explains the smaller amplitudes of the GFs corresponding to the shorter wavelengths in decomposition of basic blue and green GFs. To interpret broader GFs in the decomposition at the tails of basic blue and green GFs further investigation is needed.

Basic blue and green GFs can be also treated as separate spectra emission from blue and green QWs which makes it possible to evaluate spectral distributions of the number of extracted photons associated with emission from blue and green QWs.

Dependencies of the fractions of extracted blue and green photons in the total number of extracted photons versus total injected current are shown in Fig. 5. One can see from Fig. 5 that increase in injected current results in the increase of the fraction of blue photons while fraction of green photons decreases. It should be pointed out that the number of extracted photons is proportional to the number of generated photons. In the planar LED structure under consideration, the holes from p-doped region first reach green QWs and recombine there. Then the rest of them can be captured in the blue QWs. Thus, the larger number of holes can reach blue QWs with increasing forward bias voltage and injected current. It worth to mention that the calculated ratios of extracted photons correspond to the splitting of the injected charge carriers between green and blue QWs.

4. Conclusion
Decomposition procedure into Gaussian functions was developed and applied to analyze EL-spectra of the blue-green LED with patterned electrode measured experimentally. In two-
step decomposition we first separated basic GFs for blue and green emission lines from the experimental EL-spectrum. Then these basic blue and green GFs were decomposed into the sets of secondary GFs. FWHM of the most secondary GFs in each set is close to the value determined by thermal broadening. Extraction of narrow “secondary” GFs can be useful to relate broadening of the observed EL-spectra to the impact of mesh-like electrode. Analysis of basic GFs allows also to assess the splitting of the injected charge carriers between QWs for green and blue emission.

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