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Short Communication

# Emission band width approximation of light-emitting diodes in the region 350–2100 nm

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ABSTRACT

Emission spectrum of a light-emitting diode (LED) exhibits essential broadening as its central wavelength grows. This effect has been modeled in the visible and near infrared region (350–2100 nm) using a library of 76 digitized LED spectra approximated by the Gaussian function. The emission peak width expressed as the Gaussian full width at half maximum (FWHM) was shown to follow a second-order polynomial dependence on the central wavelength. Suggested approximation principles enable the reproduction of realistic emission spectra of LEDs based on their central wavelength only. This approach can be used for the development of LED-based optical sensors, e.g. to find the optimal number and working wavelengths of constituting LED elements, as an alternative to the exhaustive library-based optimization. The practicability of suggested modeling method was illustrated by two application cases.



## 1. Introduction

Light-emitting diodes (LEDs) are increasingly used by the modern optical technologies. In particular, LEDs are applied as nearly monochromatic light sources for optical sensors presenting a cost-effective and portable alternative to the full-range spectrophotometry [1–5]. Significant technical simplification of device is achieved due to the replacement of high-resolution spectra containing many excessive variables by a few measurements at target wavelengths optimized for a particular application. Accurate customization of a LED-based optical sensor, i.e. determining the best number and working wavelengths of the LED-sources, should be performed under consideration of their spectral properties, in particular, their emission band widths.

Optimal configuration of the LED-sensor is modeled mathematically using variable interval selection on the preliminary obtained full-spectrum data. The LED-sensor variables are obtained by the integration of spectral variables in the experimental calibration set within the LED emission region using the spectra of chosen LEDs as variable weights [3]. Two examples of the LED-sensor development are given in our previous publications. In [3] the optimal sensor configurations for simultaneous determination of fat and total protein in milk have been calculated. Seven optimal wavelengths were selected using emission spectra of 59 commercially available LEDs in the region of 400–1100 nm. Recently, a four-wavelength LED-based sensor for kidney cancer diagnostics and the respective discrimination model have been simulated using measured spectra of preselected LEDs and full reflectance spectra of the samples in the range of 900–1720 nm [4].

It was noticed [3,4] that LED emission band's full width at half maximum (FWHM) strongly depended on the central wavelengths growing from 3–7 nm in the ultraviolet region to 150–200 nm in the NIR above 1600 nm. The LED spectrum widening strongly affects the performance of analysis and thus cannot be neglected at the sensor modeling stage.

In the present work we use a representative set of the LED spectra in a wide practical range of 350–2100 nm to derive an empirical approximation function describing the dependence of the LED emission peak widths on their central wavelengths. This dependence can be used to obtain a realistic approximation of the LED spectrum at a chosen working wavelength. Continuous wavelength optimization for the sensor development is expected to be more accurate than selection of the LEDs from a limited library set.

## 2. Methods

The modeling was based on known emission spectra of 76 catalogue LEDs by Roithner LaserTechnik GmbH (Vienna, Austria) offering a large collection of semi-conductor LEDs from multiple world producers and providing a dense coverage of a wide range

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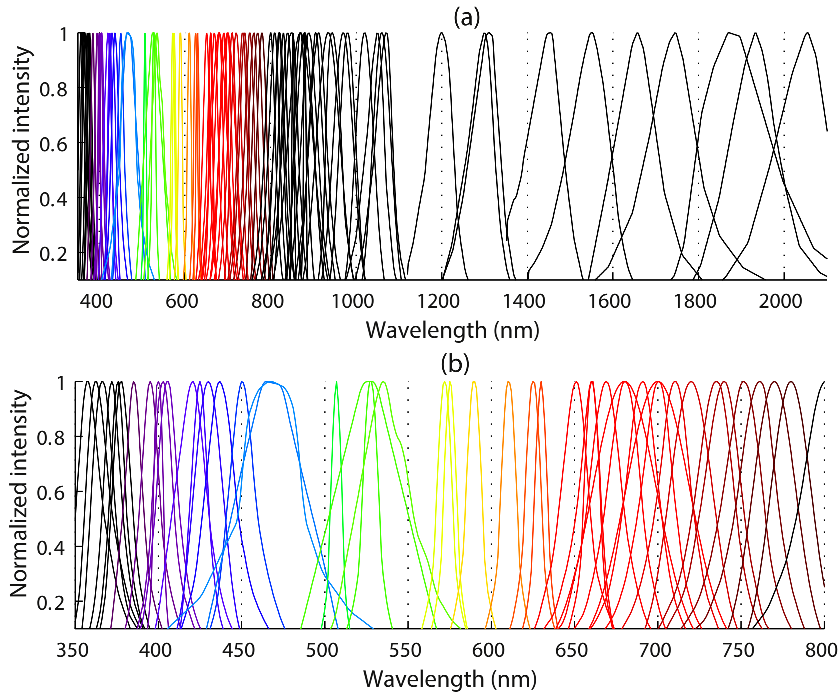


**Fig. 1.** Library of digitized emission spectra of LEDs: (a) 76 spectra in the region of 350–2100 nm. (b) 44 spectra in the region of 350–800 nm.

of emission wavelengths (λ) [6,7]. The spectra were obtained by means of computer-aided digitization of images in the LED technical documentation using a home-made software. The digitized spectra were initially read-in and saved as piece-wise linear functions between the pin points selected by an operator that were further interpolated to the standard grid of 1 nm. The λ-axis was assigned using two end points of the spectral image (Fig. 1).

Fig. 1 The bell-shaped emission spectra of LEDs can be described by the Gaussian function, assuming the normal distribution of emission energy [8]:

$$S(\lambda, \lambda_{max}) = exp^{-0.5\frac{(\lambda-\lambda_{max})^2}{0.18\cdot w(\lambda)^2}} \quad (1)$$

where $S$ is the normalized spectral intensity, $\lambda_{max}$ – the central emission wavelength, and $w$ – FWHM. The Gaussian variance parameter is the peak FWHM multiplied by $\sqrt{0.18}$ ($\sigma = \frac{w(\lambda)}{2\sqrt{2ln2}} \approx \sqrt{0.18}\cdot w(\lambda)$). The $w$ ($\lambda_{max}$) function was derived by the least-squares fitting of all pairs of FWHM and $\lambda_{max}$. values from the LED library.

The root mean-square error (*RMSE*) was used to assess and minimize the approximation error between digitized and approximated LED spectra (Eq. (2)).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{k}\left(\hat{y}_i - y_i\right)2k}{}} \quad (2)$$

where $y_i$ and $\hat{y}_i$ are respectively digitized and Gaussian intensities above the threshold of 0.1, and $k$ is the number of approximated points. *RMSE* was also used to characterize the fitting of FWHM dependence on $\lambda_{max}$ by suggested polynomial function. In that case $y_i$ and $\hat{y}_i$ were known ($w$) and estimated FWHM of $k$ LEDs.

Data analysis was performed in MATLAB R2008b (The MathWorksTM Inc., USA). PLS regression [9] models with the data weighting by LED spectra were built in Interval Selection Toolbox for GNU Octave (version 3.6.4, https://www.gnu.org/software/octave/index.html) and using web-based chemometrics software TPT-cloud (www.tptcloud.com) by Global Modelling (Germany) and Samara State Technical University (Russia).

## 3. Results and discussion

There is a pronounced growth of the LED emission band width with the wavelength (Fig. 1) that is technically explained by injection electroluminescence physics [8]. This phenomenon should be taken into account at the development of precise optical sensors.

The following polynomial function has been suggested to describe the wavelength dependence of FWHM:

$$w(\lambda) = 4.1909\cdot10^{-5}\cdot\lambda^2 + 8.5432\cdot10^{-4}\cdot\lambda - 7.9570 \quad (3)$$

The polynomial order was chosen based on the comparison of FWHM approximation *RMSE* values (Eq. (2)). Different polynomial approximations are presented in Fig. 2. The linear dependence is evidently biased and the corresponding *RMSE* = 15.8 nm is too high, while the third and fourth order polynomial functions fit the data with a similar quality (*RMSE* of 13.28 and 13.29 nm, respectively). Following the principle of simplicity, the quadratic polynomial was preferred (*RMSE* = 13.9 nm).

Fig. 2 Analytical approximation of FWHM can be used to test hypothetical LEDs in the course of sensor modeling. A LED spectrum for any λ is then calculated by substituting of estimated $w$ (Eq. (3)) into Eq. (1).

Desirable LEDs resulting from the sensor optimization have realistic spectral properties and thus can be easily acquired. Optimization based on the hypothetical (but realistic) instead of preselected LED spectra presents an improvement potential for the sensor performance. Otherwise, the development is limited to library diodes that can be non-optimal [3].

Feasibility of the subsequent transfer from hypothetical to real LEDs is illustrated in Fig. 3. One can see that Gaussian function suits well for the approximation of seven library LEDs selected for the sensor in [3]. The Gaussian peaks calculated by Eq. (3) at the same wavelengths in most cases closely reproduce the real LED spectra.

Fig. 3 Suggested approach was tested using the data of milk fat and protein determination [3], where a seven-LED sensor in the