Influence of the quantum well models on the numerical simulation of planar InGaN /GaN LED results

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Abstract. Within this paper, we present electric model of a light emitting diode (LED) made of gallium nitride (GaN) followed by examples of simulation results obtained by means of Sentaurus software, which is the part of the TCAD package. The aim of this work is to answer the question of whether physical models of quantum wells used in commercial software are suitable for a correct analysis of the lateral LEDs made of GaN.

1. Introduction

Numerical simulations are the tool that is often used to investigate and optimise new semiconductor devices. This approach is especially useful when the semiconductor devices that must be characterised by the special dimensions and sophisticated design. The CAD packages basing on physical description of phenomena taking place in semiconductor structures are an effective tool both at the stage of new devices design and optimisation of their parameters. There are a lot of homemade software packages that have been reported in literature, but nowadays, the application of the commercial, more universal ones is preferred. Among such packages, present on the market, one should mention Atlas-Silvaco, tiberCAD-TiberLab, Medici-Synopsys, GTS-GlobalTCADSolutions and Sentaurus. The latter one has been chosen as a numerical tool for the investigation presented in the paper.

Sentaurus package, initially, has been designed as a CAD tool for silicon technology. Next, following the progress in microelectronics, it was adopted for other materials and updated by models introducing new phenomena e.g. quantum effects. The modifications enlarged the extent of the software applicability in the formal way, but the packages were still used to investigate silicon structures mainly with limited credibility to other semiconductor materials. Therefore, in order to recognise the usefulness and correctness of Sentaurus code with implemented models of physical phenomena for modelling of gallium nitride (GaN) structures, series of test simulations were elaborated. They focused on a simple real optoelectronic GaN structure. Special attention has been paid to modelling the quantum wells (QWs) appearing in the considered domains. In the Sentaurus code, QWs can be treated without any quantum corrections, like in [1], or with the aid of quantum well models available in the Sentaurus libraries [2].
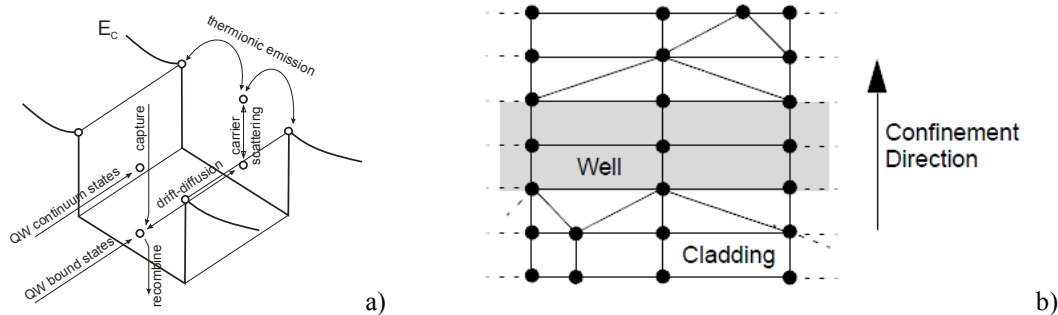
As the representative real optoelectronics GaN device for the numerical investigations, the planar InGaN/GaN blue LED structure covering MQW layer, which design and manufacturing is described in [3], has been chosen. The paper [3] presents most of the LED design data necessary for numerical model creation and the basic characteristics of manufactured device. In the investigations reported here, the

numerical models of the chosen LED structure taking into account different QW approaches have been compared. The conducted simulations allow evaluating the available in Sentaurus QW models.

2. Numerical Models of QW

In the Sentaurus package, there are implemented two different physical models of quantum wells. The first *QWTransport* is based on a specific approach to the area of quantum well (QW). This area is considered as a point source of recombination [2, 4]. This assumption leads to a simplification of the phenomena occurring inside the QW, and forces the creation of an appropriate discretization grid, as shown in figure 1.

Figure 1. Discretization of quantum well according to Sentaurus *QWTransport* rules
(physical phenomena – a, discretisation mesh – b)

Let us consider two cases of carrier transport by the quantum wells. In the case of transport perpendicular to the QW plane, the QW is preserved as a point source of recombination, which contains separate continuum and bound states. In this case, the continuum and bound states are assumed to have different quasi-Fermi levels that lead to separate continuity equations for the continuum and bound states. Transport of carriers from the regions outside the QW to the QW continuum states is by thermionic emission. The transition from the QW continuum to the bound states is computed by a scattering rate that includes carrier–carrier scattering. The bound states are solved from the Schrödinger equation. In the case of transport in a direction parallel to the plane of the QW, it is simulated basing on drift-diffusion model.
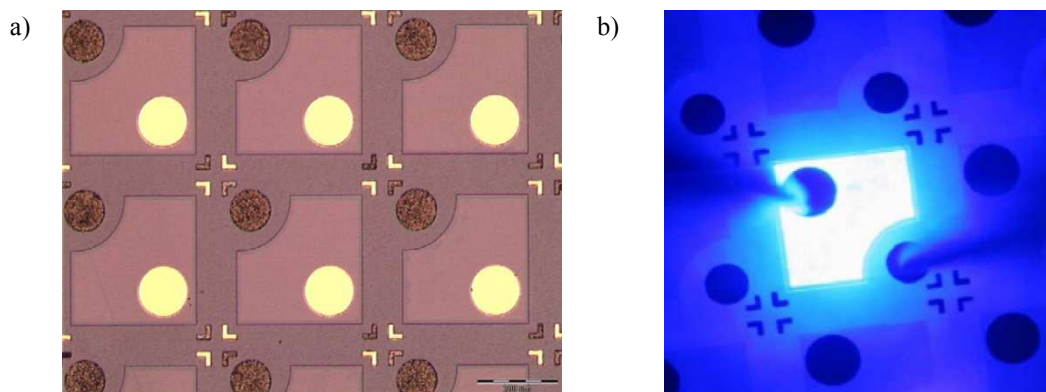
This approach determines a special mesh generation. The grid is based on the 'three points' model. It specifies that only one node of the mesh is placed in the centre of the well while the other two, respectively, at the edges of the QW region. This principle is schematically shown in figure 1b. Disadvantage of this approach is that there is no possibility to analyse the structures in which the QW regions are not perpendicular to the direction of carriers transport or when the QW region has more than one plane. The solution to the above mention problem is the application of another model – *QWLocal* [2]. From a technical point of view, this model does not require exactly 3 nodes in the quantum well. It is also possible to model structures in which the quantum wells can be arranged in different planes. This model has only one condition. The area of quantum well should be the same throughout the semiconductor structure.

In opposite to the *QWTransport* model in the *QWLocal* model, there are not designated carrier density corresponding to the status related to the quantum well. The carrier concentrations in the quantum well, as in the *QWTransport* model, are based on one-dimensional Schroedinger equation of energy levels - thereby modifying classically calculated carrier concentrations. The amount taking into account energy levels to analyse occurrence, is equal to: the sub-bands for electrons: 5, sub-band for light holes: 4, sub-bands for heavy holes: 2, sub-bands for the hole resulting from cleavage originating from the crystal field: 2, the amount of valence band: 3, respectively. In the case of LED modelling,

there is no stimulated emission and spontaneous emission that takes into account the presence of the aforementioned sub-bands.

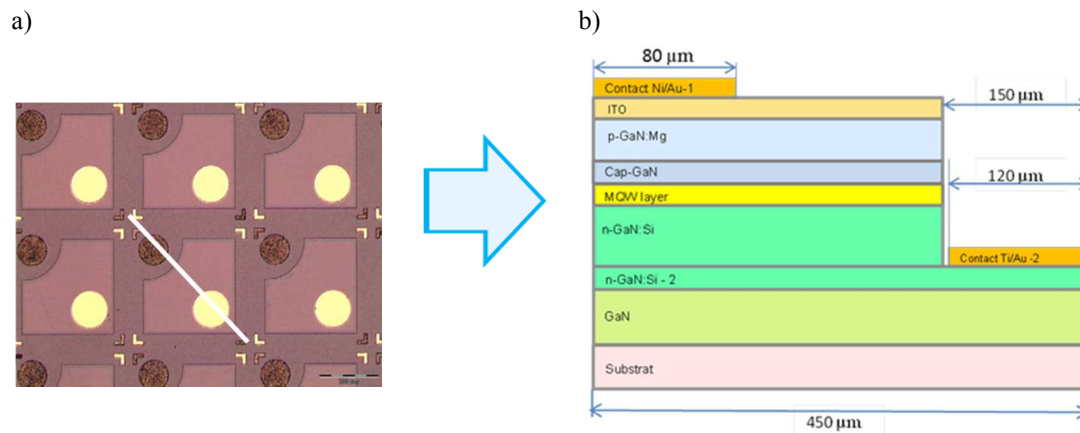### 3. Modelling of Real GaN LED Structure

The models presented above confirmed that in general, we are able to use the Sentaurus package as the base to model phenomena taking place in optoelectronics GaN structures. We decided to perform simulations of a real GaN blue LED described in the literature [3]. The chosen structure is shown in photographs [3] in figure 2 presenting several chips on one wafer and the blue light emitted from one of the fabricated chips, respectively.

Figure 2. Photographs of several LED chips (a) and blue light emitted from one of the fabricated LED chips (b) [3]

It is a planar rectangular structure with dimensions 315 x 315 μm^2 and two round contacts placed along the diagonal at opposite corners of the structure, as it is sketched by the white line in figure 3a. The diagonal represents the simplest way for the current flow from anode to cathode, characterised by the lowest electrical resistance. It means that in the plane defined by the white axis, the direction of the anode-cathode current exactly agrees with the direction of the white axis and its flow can be considered as 2D phenomenon. It has allowed to develop a 2D model for its investigation, in which, the numerical simulations are carried out for the 2D domain corresponding to plane defined by the white axis. The layers that have been distinguished in the 2D domain together with their lateral dimensions are shown in figure 3b.

The sample LED consists of several layers. These include: sapphire substrate, GaN buffer layer, Si-doped n-GaN layer, multi quantum wells layer, cap GaN layer and Mg-doped p-GaN layer. The design data necessary to develop the numerical model of considered structure has been taken from the study [1] mainly and completed on the base of literature research. They are collected in table 1. Not all the layers listed in the table have finally been taken into account in the developed model. It covers the layers 3-7 only. The contact layers 1-2 and 10 have been replaced by ideal contacts whereas the layers 8-9 have been removed due to their negligible participation in the anode-cathode current flow.

a)   b)

Figure 3. LED structure: (a) and the top view of the diagonal location on the considered chip [3], and (b) 2D domain corresponding to the diagonal plane
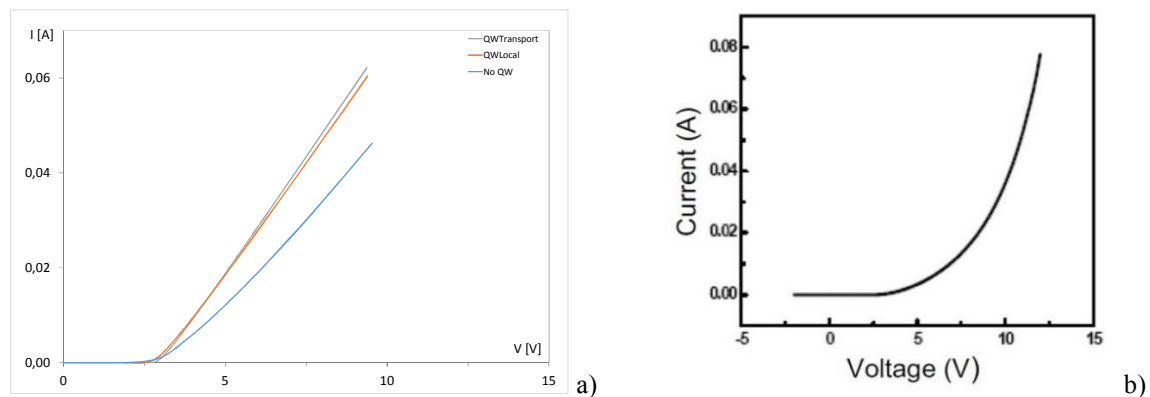
Table 1. Data describing the considered real GaN blue LED structure

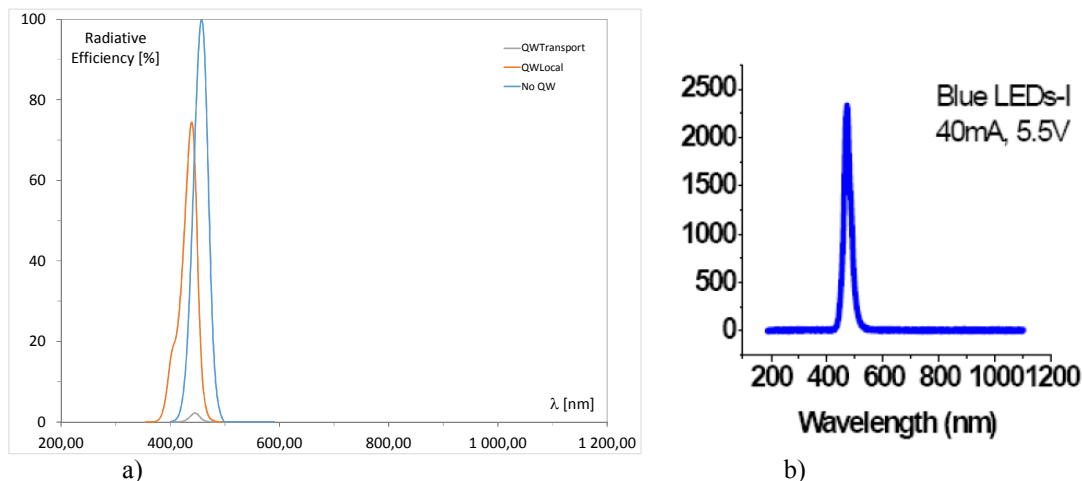|	Layer	doping [cm^{-3}]	thickness [nm]
1	Contact-Ni/Au1	-	200
2	ITO	-	100
3	p-GaN:Mg	$8 \cdot 10^{17}$	250
4	Cap-GaN	$1 \cdot 10^{16}$	30
5	MQW 3 pairs In$_{0,4}$Ga$_{0,6}$N GaN barrier	$1 \cdot 10^{16}$	39 3 10
6	n-GaN:Si	$8 \cdot 10^{18}$	700
7	n-GaN:Si-2	$8 \cdot 10^{18}$	300
8	GaN		
9	Substrat		
10	Contact Ti/Au2		

4. Results

The worked out model has been used for isothermal (T=300K) simulations that run successfully. Simulations were conducted using both previously described models of quantum wells. For comparison, performed simulations also took into account the models of classical physics. The main aim of these simulations was to determine the basic parameters characterising the device, such as threshold voltage, the resistance in conducting state and the wavelength of the emitted radiation. The first two parameters were determined from the current-voltage (IV) characteristic, while the last from the emission characteristic. Both these characteristics are shown in figure 4a and figure 5a, respectively.

The first simulations were performed for the *QWTransport* model. Assuming the composition of In$_{0,4}$Ga$_{0,6}$N, compatible with the literature data [3] we obtained the maximum luminous intensity for wavelength $\lambda = 545$ nm and not as expected for 450 nm. Therefore, new fraction of the InGaN was calculated to fit the expected wavelength, assuming that the radiative recombination occurs only in quantum wells. For the final simulations we used the new ratio of indium fraction, which was 0.2. The same factor was used for subsequent simulations with other physical models (*QWLocal* and *NoQW*).

Figure 4. Comparison of simulated (a) and measured in [3]
(b) I-V characteristics of considered GaN LED structure

Figure 5. Comparison of the electroluminescence spectra resulted from numerical simulations (a) and
measured in [3] (b) of considered GaN LED structure

Some of the results that have their counterparts in the measurement results presented in [3] are compared in figure 4 and figure 5. In the first case, the I-V characteristics, calculated as isothermal ones, are juxtaposed with the characteristic measured in non-isothermal conditions whereas in the second case the electroluminescence spectra are compared. Moreover, three extracted parameters from the above characteristics for three approaches are gathered in table 2. The threshold voltages V_T for numerical simulations are determined based on the linear approximation of I-V characteristics, while the wavelengths λ are defined as the maximum of the radiative efficiency spectrum. The measured values are taken from [3].

The similarity of numerical and experimental results is evident, e.g. the wavelength corresponding to the maximum of electroluminescence obtained numerically and experimentally are 440 nm or 445 nm and 466,5 nm, respectively. Full width at half maximum (FWHM) parameter, that allows determining the selectivity of the emitted signal in whole spectrum, is similar for *QWLocal*, *NoQW* approaches and the measured characteristic. Unfortunately, *QWTransport* suffers from unexplained emission suppression. Furthermore, the threshold voltage values obtained numerically and experimentally are comparable. The difference in the shape of the I-V curve can be caused by the fact that the numerical simulations were carried out under isothermal conditions (T = 300 K). It was not possible to determine

the real measurement thermal conditions from [3]. The second factor that can influence the IV characteristic shape is the construction of the numerical structures and the real LED. The models do not include ITO current spreading layers. Removal of this layer affects the current distribution inside the structure, and in consequence current densities on contacts. In figure 5a, we can see that the *QWLocal* peak broadens. This is due to the occurrence of radiative recombination in the GaN structure on p-n junction, outside the multi-quantum wells region. Nevertheless, both types of presented characteristics show that the two tested quantum models behave similarly. The emission suppression in the case of *QWTransport* approach needs further investigations.

Table 2. Characteristic parameters InGaN LED obtained from simulation and measurements

	QWTransport	QWLocal	NoQW	measured
V_T [V]	3,2	3,1	3,5	4 [3]
λ [nm]	445	440	458	466,5 [3]
FWHM [nm]	20,7	29	31	~30

5. Conclusions

The paper focuses on verification of quantum models embedded in Sentaurus TCAD package. The main aim was to point out the most suitable approach to analyse optoelectronic GaN devices with quantum wells. The two models were tested. The results obtained using these models are comparable with the results obtained for the real LED [3]. Although both models behaved similarly while performing electrical analysis, the optical analysis of *QWTransport* model suffers from unexplained emission suppression. Moreover, *QWTransport* model has a very big disadvantage connected with specific requirements on grid generation. Hence, the *QWLocal* model should in the area of interest in the case of optoelectronic GaN device analysis.

In the case of commercial software, like Sentaurus, the user should pay attention the data delivered with built-in material libraries. The parameters defined in them may differ from the values given in other sources a lot. It may reflect the obtained results, so one should not treat them uncritically.

6. References

[1] Saguatti D, Bidinelli L, Verzellesi G, Meneghini M, Meneghesso G, Zanoni E, Butendeich R, Hahn B, 2012 *IEEE Trans. on Electron Devices* **59(5)** 1402-1409
[2] Sentaurus Device, User Manual, Ver. J_2014.09
[3] Nguyen X L, Nguyen T N N, Chau V T and Dang M C 2010 *Adv. Nat. Sci.: Nanosci. Nanotechnol.* **1** 025015 (5pp)
[4] Grupen M, Hess K 1998 *IEEE Journal of Quantum Electronics* **34(1)** 120-140

Acknowledgements