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Defects in InGaN QW Structures: Microscopic Properties and Modeling

Matteo Meneghini[a,b], Marco Nicoletto[a], Francesco Piva[a], Nicola Roccato[a], Alessandro Caria[a], Fabiana Rampazzo[a], Carlo De Santi[a], Matteo Buffolo[a,b], Francesca Rossi[c], Giovanna Mura[d], Andrea Gasparotto[b], Conny Becht[e], Gunnar Kusch[f], Yihong Ji[f], Xuanqui Huang[g], Houqiang Fu[g], Hong Chen[g], Yuji Zhao[g], Nicola Trivellin[h], Gaudenzio Meneghesso[a], Enrico Zanoni[a], Rachel Oliver[f], Nicolas Grandjean[j], Ulrich T. Schwarz[e]

[a]University of Padova, Department of Information Engineering, matteo.meneghini@unipd.it
[b]University of Padova, Department of Physics and Astronomy
[c]CNR IMEM, 43124 Parma, Italy
[d]University of Cagliari, 09124 Cagliari, Italy
[e]Chemnitz University of Technology, 09126 Chemnitz, Germany
[f]Cambridge University, Cambridge CB3 0FS, United Kingdom
[g]Rice University, Houston, TX 77005 USA
[h]University of Padova, Department of Industrial Engineering
[j]Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

ABSTRACT

Defects can significantly modify the electrical and optical properties of quantum well (QW) structures based on InGaN. We present an overview of our recent results on the properties of point and extended defects in InGaN/GaN QW devices.

By analyzing single-quantum well (SQW) devices, we show that: defect density is higher in indium-containing layers; also, the use of an indium-containing underlayer can significantly reduce the density of traps in the active region of the devices, resulting in a better device efficiency. The properties of defects can be effectively extracted by deep-level optical spectroscopy.

Furthermore, by studying multiple QW samples with a high number of periods, we demonstrate that: a) extended defects, and related V-pits, may locally modify the current distribution across device area. A TCAD model has been defined for numerical simulation of conduction near V-pits. b) the presence of agglomerates of V-pits may result in a locally increased photogenerated current density; also, we identified a significant redshift in emission wavelength in proximity of agglomerates of V-pits, surrounded by trench-like defects.

This article provides a wide range of results for a better understanding of the properties of defects in InGaN/GaN devices.

Keywords: gallium nitride, light-emitting diode, defect, trap, dislocation, V-pit

1. INTRODUCTION

Over the past decades, the research in the field of nitride-based light-emitting diodes (LEDs) has shown impressive advancements. Internal quantum efficiencies (IQE) greater than 90 % have been demonstrated for blue devices [1], >75 % for green LEDs [2], and promising performance (IQE>20 %) has been recently reported for longer wavelength (red) devices [3]. Defects can significantly impact the electrical and optical properties of LEDs [4], by altering the IQE, by creating conductive paths responsible for increased leakage, by modifying the emission pattern at microscopic level, and by reducing the lifetime of the devices. The goal of this paper is to present an overview of recent case studies, carried out on both single quantum well (SQW) LEDs and multiple QW (MQW) samples with a high number of periods. Several techniques have been used in order to present a clear overview of the topic.

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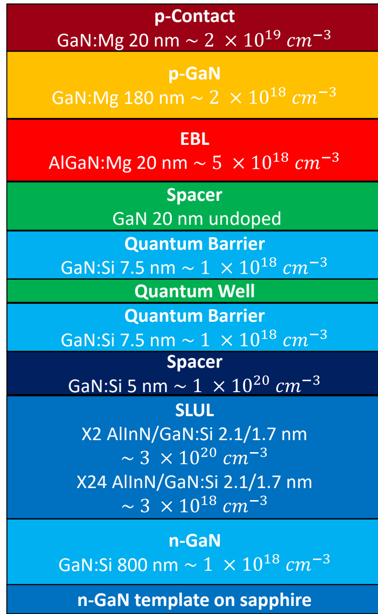
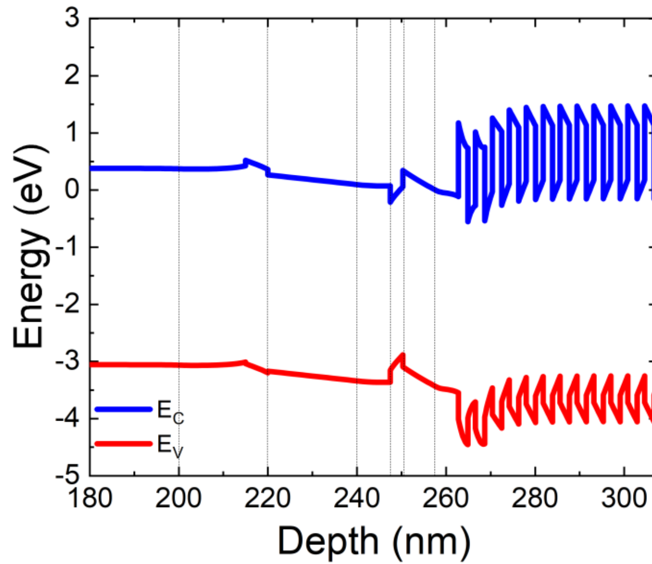
2. POINT DEFECTS: IMPACT ON EFFICIENCY

The role of point defects in limiting the IQE of LEDs was investigated by analyzing single-quantum well LEDs having the schematic structure shown in Figure 1 (a). Different splits were considered. Split A: devices with and without an indium-containing superlattice underlayer. Split B: devices having different indium content (12 %, 16 &, 20 %) in the QW. Figure 1 (b) reported the simulated band diagram for one of the analyzed devices, with a 20 % indium content in the QW.



(a)



(b)

Figure 1: (a) schematic structure of one of the analyzed SQW devices; (b) simulated band diagram (at 3 V) for one of the analyzed devices (20 % indium content in the quantum well)

The main properties of defects (density, thermal ionization energy, optical ionization energy) were extracted by means of deep-level optical spectroscopy. This technique (described in detail in Ref. [5]) is based on the measurement of the capacitance transient of a junction subject to monochromatic illumination. The results of the analysis demonstrated that: a) LEDs with indium-containing underlayer have a much smaller density of defects within the active region (Figure 2 (a)); b) even in presence of an underlayer, some defects are propagated to the active region (Figure 2 (b)); c) the density of point defects in the active region increases with increasing indium content in the QW (Figure 2 (b)). Such results were interpreted by considering that the presence of indium favors the incorporation of defects, and that an In-containing underlayer can suppress the propagation of defects towards the active region. Hypotheses on the role of the involved defects were formulated, based on the comparison with literature on the topic. Vacancy complexes and divacancies were proposed as responsible for non-radiative recombination in III-N structures[6], [7], [8].

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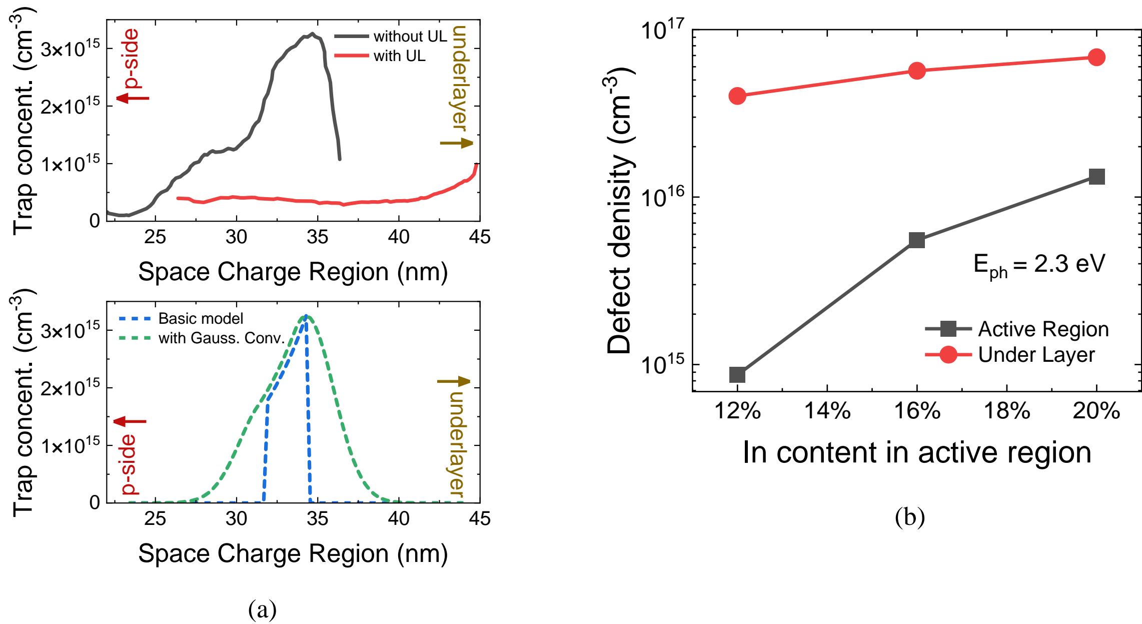

Figure 2: (a) (top) trap density profile in the QW region for LED with and without an indium containing underlayer and (bottom) modeled trap profile (for these LEDs, indium content in the QW is 10 %); (b) trap density in the active region and in the underlayer for LEDs with different indium content in the QW.

3. MULTIPLE QUANTUM WELL SAMPLES WITH A HIGH NUMBER OF PERIODS

Further analysis on the impact of defects was carried out by studying multiple quantum well samples with a high number of periods. The structure of the analyzed devices is described in detail in Ref. [9], and consists of a 30-period multi-quantum well (MQW) structure, where the barrier thickness is 7 nm, and the QW thickness is 3 nm. Indium content in the QW is equal to 15 %.

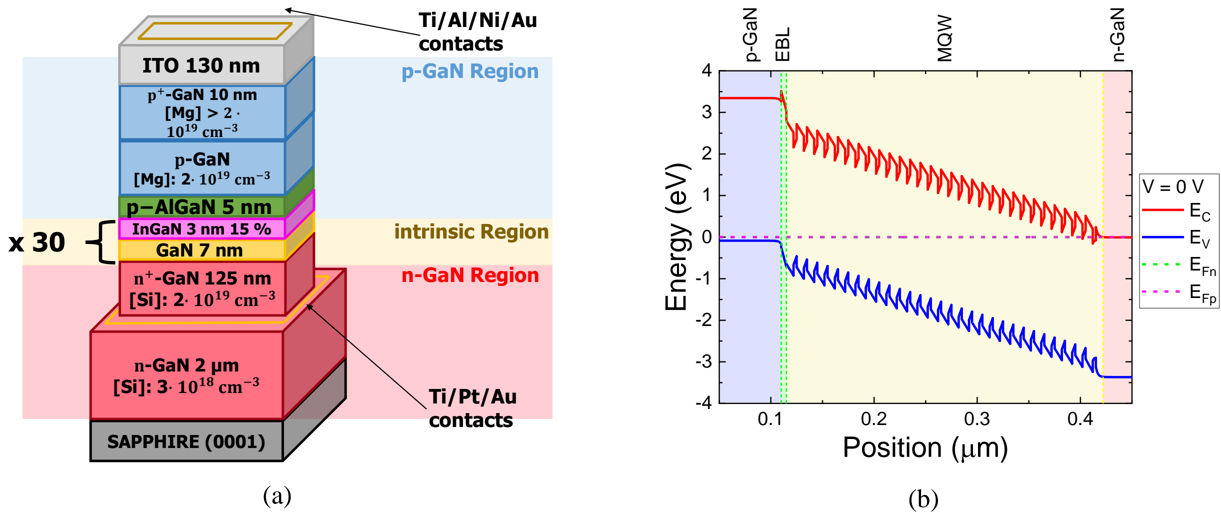

Figure 3: (a) structure of the analyzed multiple quantum well samples with a high number of periods; (b) schematic band diagram of the analyzed devices

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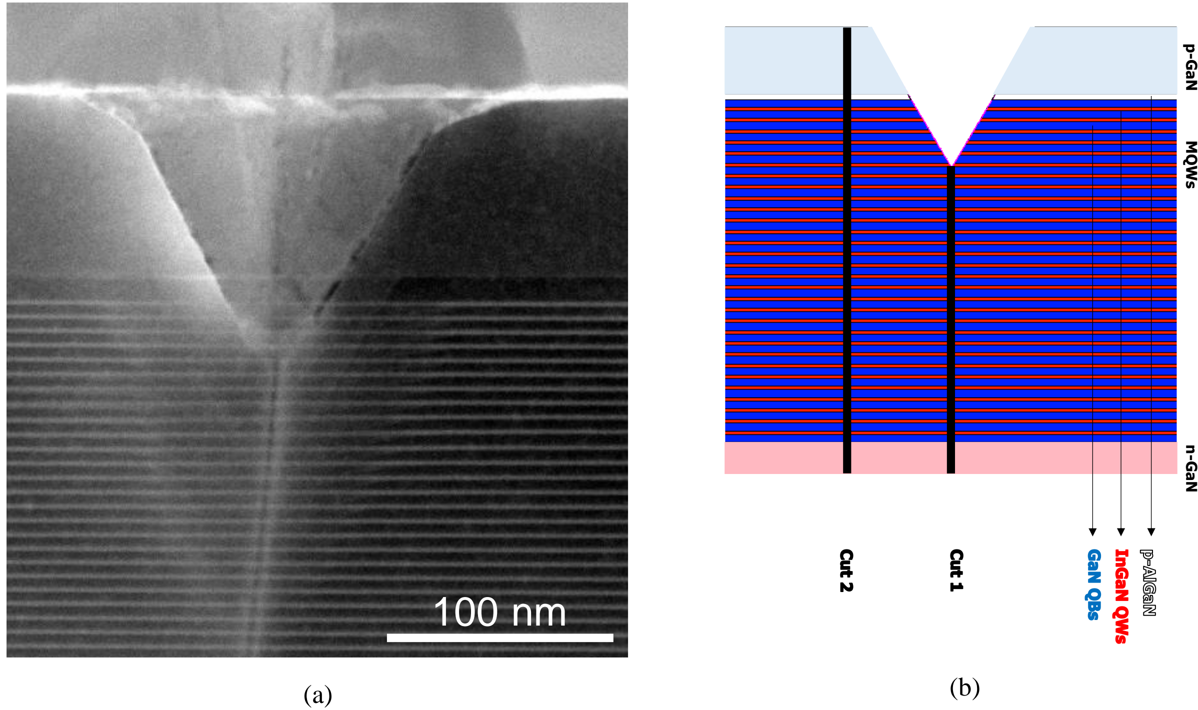
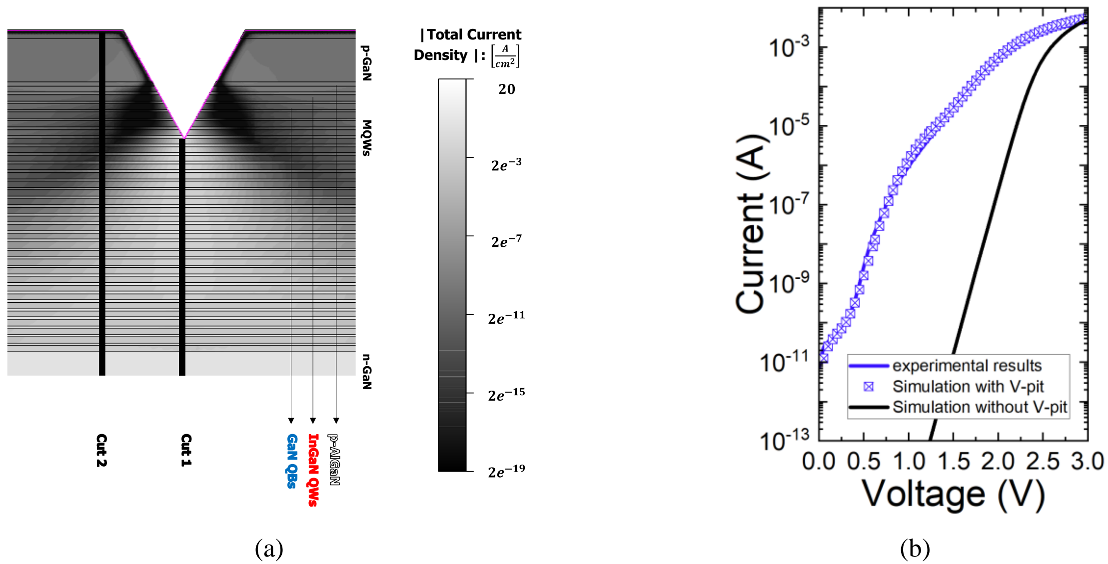
Transmission electron microscopy analysis revealed the presence of V-pits, i.e. 3D defects having the shape of an inverted pyramid (Figure 4 (a)). Such V-pits penetrate the MQW region, thus altering the conduction on a local scale. A 2D simulation model was developed, in order to describe and explain the impact of V-pits on conduction (Figure 4 (b)). For the simulations, the V-pit density was defined by fixing the ratio between the base of the pyramid (V-pit) and the size of the simulated cell. The piezoelectric charge on the V-pit sidewalls was adjusted to take into account the lower charge activation [10]. 2D simulations (Figure 5 (a)) indicated that the presence of a V-pit can significantly increase the (local) current density [11], [12]. By adding the V-pit to the LED model, the simulations were able to accurately reproduce the current-voltage characteristics of the devices (Figure 5 (b)).



(a) (b)

Figure 4: (a) TEM micrograph of one of the V-pits; (b) V-pit region as modeled in a TCAD simulator



(a) (b)

Figure 5: (a) simulated current density in proximity of a V-pit; (b) simulated current-voltage characteristic of one of the MQW devices, including the effect of V-pits

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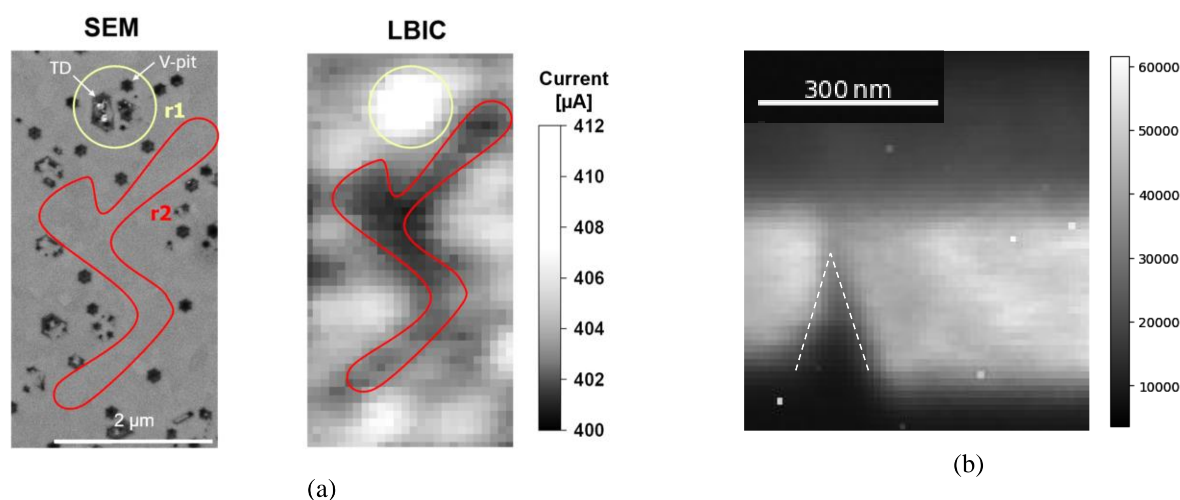
Further analysis was carried out in proximity of V-pits identified by scanning electron microscope (SEM) micrographs. Figure 6 (a) shows a picture of the surface of one of the analyzed samples, highlighting some reference regions. The same figure also reports the results of light-beam induced current (LBIC) measurements carried out on the same device area [13]. As can be observed, the photo-generated current shows an increase in the regions including agglomerates of V-pits (region “r1”), which are then more conductive than the V-pit free regions (region “r2"). It is worth noticing that region “r1” has a brighter LBIC signal possibly because it includes (besides isolated V-pits) also a trench defect (TD, opening to the surface as a set of coalescing pits [11]). At the same time, cross-sectional cathodoluminescence (CL) analysis carried out on lamellas in a SEM setup (Figure 6 (b)) indicated that the regions near the trench defect have a much lower radiative efficiency, and appear as dark-spots. It is worth noting that Figure 6 (b) exemplifies the use of CL in cross section to study V-pits and trench defects, a technique on which we plan to write further in future.

Finally, we found a significant redshift in emission wavelength in proximity of agglomerates of V-pits, in presence of trench-like defects [13]. This result was explained by considering that agglomerates of V-pits and related trench-like complexes can result in a higher indium incorporation. This results in a longer emission wavelength, compared to defect-free materials.



(a)

(b)

Figure 6: (a) (left) SEM micrograph and (right) light-beam induced current in an area rich of V-pits; (b) cathodoluminescence pattern measured on a lamella in a SEM, in proximity of a trench defect

4. CONCLUSIONS

We presented an overview on the properties of point and extended defects in LEDs based on III-N semiconductors. Several aspects were discussed, including: a) the incorporation of defects in In-containing layers, and the related characterization techniques; b) the dependence of point defect density on indium concentration; c) the impact of V-pits on parasitic conduction, and an approach to model the same by means of TCAD; d) experimental data on the increased current and reduced optical efficiency in proximity of V-pits. The results presented in this paper provide a better understanding of the properties of point and extended defects in InGaN-based light-emitting devices.

ACKNOWLEDGEMENTS

This study was developed in the framework of the research activities carried out within the Project “Network 4 Energy Sustainable Transition—NEST”, Spoke 1., Project code PE0000021, funded under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.3— Call for tender No. 1561 of 11.10.2022 of Ministero

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dell'Universita` e della Ricerca (MUR); funded by the European Union—NextGenerationEU. The CL facility was funded by EPSRC under EP/R025193/1.

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