STUDY OF CATHODOLUMINESCENCE IN InGaN/GaN NANOSTRUCTURE BY MONTE CARLO METHOD

J. Priesol[1], A. Šatka[1], P. A. Shields[2], D.W.E. Allsopp[2], D. Donoval[1] and F. Uherek[1]

[1] Slovak University of Technology, Faculty of Electrical Engineering and Information Technology, Ilkovičova 3, 812 19 Bratislava, Slovakia

[2] University of Bath, Department of Electronic and Electrical Engineering, Claverton Down, Bath BA2 7AY, United Kingdom

E-mail: juraj.priesol@stuba.sk

Received 30 April 2011; accepted 15 May 2011.

1. Introduction

In this paper, luminescent properties of InGaN/GaN single quantum well (QW) light emitting diode structures grown on the facets of GaN nano-pyramid arrays were studied by spatially and spectrally resolved room temperature cathodoluminescence (CL). Quantitative interpretation of CL measurements has been performed using Monte Carlo (MC) method. For these studies, MC simulator programmed in MATLAB has been developed, which allows modeling of an interaction of accelerated primary electrons with the solid matter using mathematical algorithms based on random change of direction and magnitude of scattering, previously studied by [1-4] and others.

2. Experimental

Room temperature CL measurements were performed in FEG SEM LEO-1550 using optical collection system with spectral range 200-2000 nm, consisting of elliptical mirror in the microscope chamber which directs emitted light from the sample towards an external collimator. Photomultiplier with narrow-band optical filter has been used for measurement of spectrally-resolved CL maps and optical fibre spectrophotometer for CL spectra.

3. Results and discussion

Fig. 1a) shows the ordered array of GaN nano-pyramids with InGaN/GaN QWs grown on the GaN facets. Height of nano-pyramids is ~300 nm and typical period of the array is 460 nm. Corresponding Integral cathodoluminescence (ICL) map obtained at acceleration voltage of U_{pe} = 3 kV is shown in Fig. 1b). Collected map reveals very low ICL signal from the top of pyramids, whilst the rest of the surface of nano-pyramids shows relatively high luminescence.

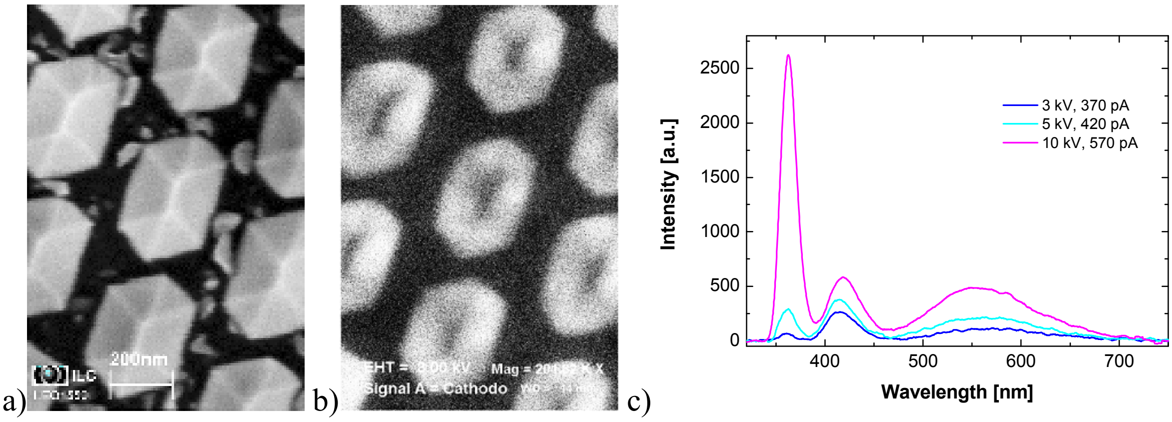


Fig.1: *a) SEM image of GaN nano-pyramids with InGaN/GaN QWs on the facets, b) corresponding ICL distribution at U_{pe} = 3 kV, c) CL spectra taken at various acceleration voltages [5],[6]*

Fig. 1c) shows the CL spectra of the sample recorded at U_{pe} = 3, 5 and 10 kV from the facet of the pyramids. Three typical peaks can be observed – a sharp emission peak at ~365 nm associated with GaN, middle peak centered at ~415 nm associated with InGaN QWs and a broad band with the maxima at ~550 nm corresponding to deep levels in GaN. It is evident, that the total signal from the sample increases with increasing acceleration voltage, although this increase is not uniform for whole spectral range. For example, near band edge GaN peak strongly increases with acceleration voltage, whilst the signal from InGaN QWs increases very slightly.

Qualitative in-depth study of the phenomena has already been published in [5] and [6], but quantitative study is still missing. MC simulation has been used for quantitative assessment of the contribution of individual parts of the nano-pyramid QW structure to CL signal. The cross-section of a single nano-pyramid used in simulations is schematically illustrated in Fig. 2a). Simulated trajectories of the first 200 electrons of electron beam at U_{pe} = 3 kV in the facet of nano-pyramid are shown in Fig. 2b). Simulation was executed for 10^4 primary electrons using models described in detail in [7] and [8]. At the same time, random diffusion of generated

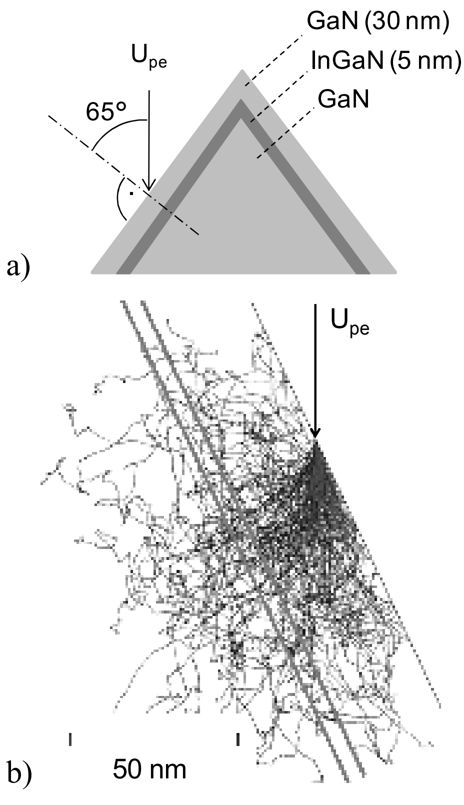
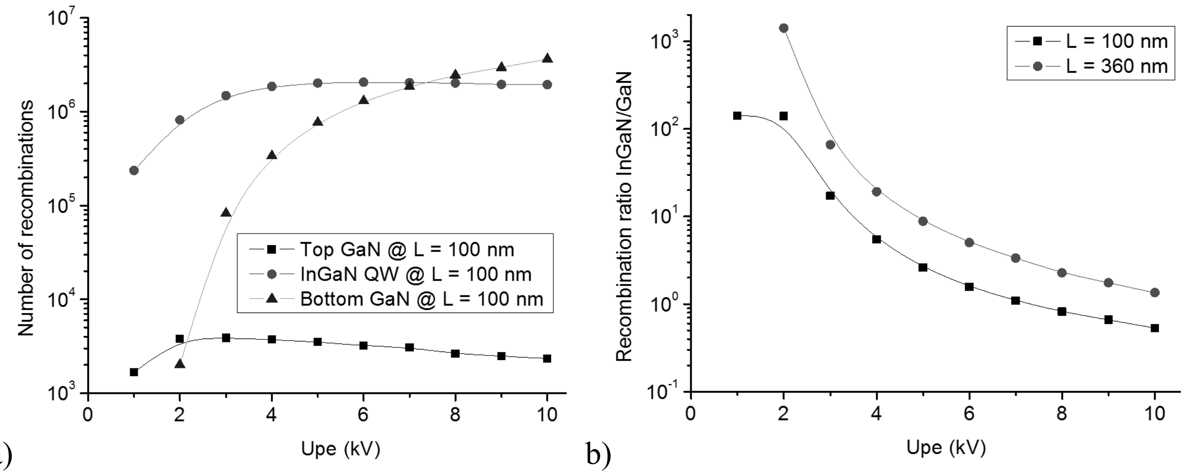


Fig.2: *a) Cross section of single nano-pyramid used in MC simulations, b) 200 simulated electron trajectories at 3kV*

charge carriers from each point of interaction between primary electrons and the sample was simulated. It was assumed, that each carrier randomly crosses k times a constant distance ds. After passing the distance $k \cdot ds$, the carriers were considered to be recombined. These parameters were estimated during simulations to approach the simulated data to the real value of diffusion length in such nanostructures. Finally, the simulations were performed for diffusion length of ~100 nm, with corresponding parameters $k = 500$ and $ds = 5$ nm. During the simulations, all recombinations were assumed as radiative, where contribution of non-radiative recombinations to the CL spectra has been neglected.



a) b)

Fig.3: *a) Simulated dependence of number of recombinations on U_{pe} in different parts of InGaN/GaN QW nano-pyramid structure for L = 100 nm, and b)simulated dependence of the ratio of CL signal from InGaN QW to GaN surrounding layers on U_{pe} for L = 100 and 360 nm*

The dependencies of number of recombinations on acceleration voltage U_{pe} for different parts of the nano-pyramid structure are compared in Fig. 3a). At the first glance, the lowest signal arises from 30 nm thick top GaN layer with the maxima at ~3 kV. The luminescence from QW increases with increasing of U_{pe}, reaches the maxima at ~6 kV and then very slowly decreases, because of longest mean free path of primary electrons at higher energies. On the other hand, the measurements in Fig. 1c) show a slight increase of InGaN peak with increasing of U_{pe}. It can be also seen, that CL signal from surrounding GaN regions is smaller than from InGaN at the voltages below ~7 kV, where at least half of all generated carriers is trapped by 5 nm thick InGaN QW during their random diffusion. Measurements and simulations for U_{pe} above ~7 kV show stronger signal from GaN than from InGaN due to increasing of penetration depth of primary electrons. At $U_{pe} = U_0 =$ ~7 kV, signal from InGaN is equal to the signal from GaN. Fig. 3b) shows simulated dependence of InGaN/GaN recombination ratio on the U_{pe}, i.e. the ratio of CL signal from InGaN to CL signal from GaN for diffusion lengths 100 and 360 nm. For larger diffusion lengths, more generated carriers reach the QW region what leads to increase in CL signal from InGaN. This causes also the shift of U_0 towards higher acceleration voltages. This knowledge is of practical importance, when the diffusion length in such heterostructure is unknown. The estimation of its real value can be provided from the comparison of U_0 obtained from measurements and MC simulations of InGaN/GaN recombination ratio for various diffusion lengths. When comparing the simulations with measurements of CL spectra, slight deviations can be observed. These can originate from considering of defect-free material, from inaccuracies in used models etc.

4. Conclusion

In this work, CL from periodic GaN nano-pyramid array with InGaN/GaN QWs on the facets has been quantitatively studied by MC simulations. CL spectra measured at various acceleration voltages are compared with simulations, and good quantitative agreement has been achieved. The possibility to determine the diffusion length of generated carriers in the structures like InGaN/GaN QWs using developed MC simulator in combination with CL measurements has been demonstrated.

Acknowledgement

The authors gratefully acknowledge the support from the Slovak Grant Agency projects VEGA 1/0716/09 and 1/0866/11. Also, the support from the CE ASFEU project NanoNet 2 (ITMS code 26240120018) is kindly acknowledged.

References:

[1] H. E. Bishop: *Proceedings of the Physical Society*, **85**, 855 (1965).

[2] K. F. J. Heinrich, D. E. Newbury, H. Yakowitz: Use of Monte Carlo Calculations in Electron Probe Microanalysis and Scanning Electron Microscopy, National Bureau of Standards, Washington, U.S.A. (1976).

[3] B. Akamatsu, J. Hénoc, P. Hénoc: *J. Applied Physics*, **52**, 7245 (1981).

[4] D. C. Joy: *Monte Carlo Modeling for Electron Microscopy and Microanalysis*, Oxford University Press, Inc., New York, U.S.A. (1995).

[5] C. Liu et al: *Applied Physics Express*, 2, 121002 (2009).

[6] A. Šatka et al: In: Proc. of "SURFINT-SRENII", R. Brunner (ed.), Florence, p.84-86 (2009); ISBN: 978-80-223-2723-7.

[7] J. Priesol, A. Šatka:. In: Proc. of „Fotonika 2011", Bratislava (2011), p.38-43; ISBN 978-80-970493-2-4.

[8] J. Priesol, A. Šatka: In: Proc. of "ELITECH 2011", Bratislava (2011), in print.