Determination of internal electric fields in binary GaN/AlN multi-quantum wells: experimental and *ab initio* comparative study

A. Kaminska [1,2], P. Strak [3], J. Borysiuk [1], J. Z. Domagala [1], E. Grzanka [3], M. Beeler [4], K. Sakowski [3], E. Monroy [4] and S. Krukowski [3,5]

[1] *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland*

[2] *Cardinal Stefan Wyszynski University, College of Science, Department of Mathematics and Natural Sciences, Dewajtis 5, 01-815 Warsaw, Poland*

[3] *Institute of High Pressure Physics, Polish Academy of Sciences, Sokolowska 29/37, 01-142 Warsaw, Poland*

[4] *CEA Grenoble-INAC/SP2M/NPSC, 17 rue des Martyrs, 38054 Grenoble, France*

[5] *Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Pawinskiego 5a, 02-106 Warsaw, Poland*

The built-in electric field in polar nitride structures is a consequence of a high piezo- and spontaneous polarization in these materials. The built-in electric field affects basic physical properties, i.e. causes a large red-shift of the photoluminescence and lowers quantum efficiency due to the quantum confined Stark effect.

The polarization poses special difficulties as the problem is generally not well solved, and the proposed theoretical approaches provide results which do not have experimental verification. It is known that some measurements provide data that are much different from the theoretically obtained results existing in literature. In addition, the segregation problems in ternary InGaN and AlGaN alloys may potentially lead to drastic differences in the physical properties of such layers built into the MQWs structures. Thus the optimal solution is to synthesize binary nitride MQWs systems which could be simulated theoretically and investigated experimentally. Recent progress in the growth of such structures has enabled their investigation at the level allowing for critical evaluation of theoretical data.

In this work we have studied a series of AlN/GaN multiquantum wells (MQWs) systems. The strained wells and barriers of various thicknesses were obtained by molecular beam epitaxy (MBE) growth on polar (0001) face of 65 nm GaN layer deposited on 1 μm thick AlN substrate on sapphire. They were characterized by x-ray diffraction (XRD) and transmission electron microscopy (TEM) techniques. It was shown that high quality structures were obtained.

The optical transition energies in these structures were determined by *ab intio* calculations as well as investigated by photoluminescence (PL) measurements. It was shown that the optical emission energy decreased by over 1 eV in the structures with QWs thicknesses increasing from 1 nm up to 6 nm and experimental results were consistent with theoretical predictions. Comparison of experimental data obtained by a number of different characterisation techniques with the DFT results on the same geometry structure allowed to determine directly the polarization in the AlN/GaN in nitride systems for the first time.

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