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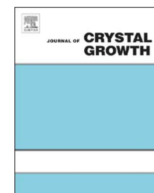

Nitride heterostructure optimization by simulation

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ABSTRACT

In current paper nanoheterostructure optimization for LED and phototransistor usage is discussed. Special doping into quantum wells and barriers by Indium atoms was investigated. By simulation improved quantum sized active region was detected which increases quantum efficiency and sensitivity upto 10%. Photoluminescence spectral curve and Peak lambda of the InGaN/GaN nanoheterostructure with different Indium concentration across wafer were investigated.

1. Introduction

$A^{III}B^{V}$ and $A^{II}B^{VI}$ nanoheterostructures (NH) and their solutions attract attention due to their unique properties. Such materials are very interesting and useful as materials for nanoelectronic devices production, e.g. Light emitting diodes (LED), photodetectors and transistors. Today, the problem of limited color range and white LEDs lack that previously prevented LED usage for general lighting have been solved, but LED/photodetectors efficiency and sensitivity need to be further improved. One of the ways to do this is the heterostructure active region optimization.

For complex optoelectronic materials and devices, especially, materials with quantum wells (QW), for LEDs and photodetectors the basic parameters that determine their quality, such as current-voltage characteristics (I–V), the quantum efficiency (QE) and photodetector sensitivity can be investigated and improved via computer simulations taking into account major structural, physical, and technological NH parameters.

2. Experimental details

At present, well-developed software packages are widely used for semiconductor materials and devices computer simulation and optimization. Some representative examples for III-Nitride devices simulation are presented in [1,2]. We, in this work, used the well known simulation package Sim Windows [3] because of its ready availability and the ease of adding new materials constants files and of additional equations files. The contribution of polarization fields was considered, as it should be in III-Nitrides. This is, of course, necessary for III-Nitrides devices due to the importance of the presence of considerable strain in the structures, the impact of polarization fields, and the importance of the quantum confined Stark effect (QCSE) [4–12]. Briefly, the main points should be noted: in the Schrödinger-Poisson equation the charges of the ionised impurity atoms, the free charge carriers and the associated charge carriers in QW are taken into account together with the polarization field and QCSE. The materials parameters for these calculations were taken from [13–20]. The growth was assumed to take place in the polar c-direction [0001]. The general view of heterostructure is shown in Fig. 1.

In the program, the expression for the three current types are used: the drift-diffusion current in the areas of the device, the thermionic emission current contacts for quantum wells with bulk materials, and the thermionic and tunneling currents at abrupt boundaries between the two bulk materials. For the charge carriers there are different recombination mechanisms: spontaneous and stimulated ones, radiative “band-band” and the non-radiative recombination mechanisms in the models of Shockley-Read-Hall and Auger are taken into consideration in the program.

In addition, for the simulation of current transport and recombination in the QW structures, LED, photodetectors special files were created. These files included the geometric dimensions of the emitters, quantum wells, and barriers; the number of quantum wells and barriers; the solid solution concentration; the conductivity type; concentration; and the impurity activation energy in each of the NH areas.

In the materials file for solid solutions, more than 25 parameters such as the band gap, refractive index, optical absorption, thermal conductivity, mobility, and lifetime of charge carriers, electron affinity, and the coefficients of radiative and non-radiative recombination were included.

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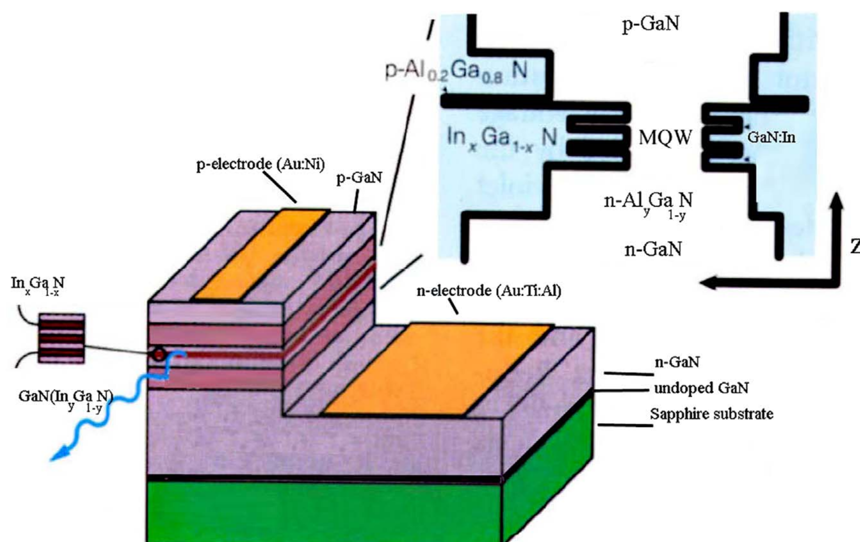

Fig. 1. Investigated InGaN/GaN heterostructure.

In current paper based on previous simulation results such as – the selected NH structure should be $p^+GaN/p^+Al_{0.2}Ga_{0.8}N/4$ (n-$In_XGa_{1-X}N$-n^-GaN)/n^+GaN with four 3.5 nm QWs and that it was also indicated that the largest contribution to the characteristics were from two central QWs and two edge QWs that act as quasi-buffers simultaneously accumulate and further inject the charge carriers [21–25] investigation for NH optimization due to impurity and Indium atoms influence in quantum active region, was carried out.

3. Results and discussion

The p–$Al_{0.2}Ga_{0.8}N$-emitter inclusion into NH is due to the needfor eliminationthe electrons injectionfrom theactive region, which is especially importantin devices simulation with low content In (X) atoms (Fig. 2).

Next, based on the optimized heterostructure, the effect of the impurity and In atoms doped into the barriers between quantum wells in the heterostructure active region was studied. This effect was represented by the nonideality coefficient dependence (Fig. 3).

Without QWs in the active area (X=0), the I-V dependence was standard. At low current densities, up to J=0.1 A/cm^2, $\eta > 1$, a significant influence on the current processes value of electrons and holes recombination in the space charge region (SCR) is observed. Then, the above-barrier-current carrier injection increasingly begins to predominate when $\eta \rightarrow 1$ at a low injection level (J=1–20 A/cm^2) and $\eta \rightarrow 2$ with increasing injection level (J=20–500 A/cm^2). The QW presence begins to affect the form of the I–V plot at values X=0.05–0.1, especially in the range of X=0.1–0.35. For X > 0.1 the value of η gradually increases over the entire range J=0.1–500 A/cm^2, reaching values of $\eta > 2$ and even higher for X > 0.15. The nonideality coefficient decreases with increasing donor impurity concentration in the barrier for the same values of X and j (Fig. 3b).

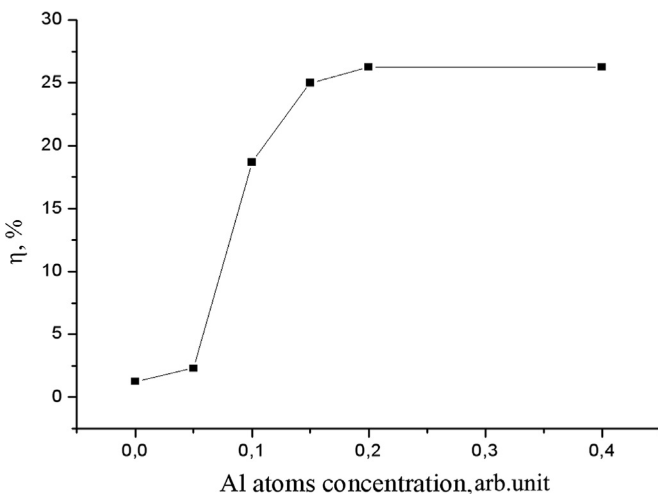

Fig. 2. Al atoms influence in the p-emitter on the InGaN LED QE.

It was detected that the optimum impurity concentration in barriers between QWs is $N_d = 10^{18}$ cm^{-3}. The QE and sensitivity increaseat the optimumAl atom concentration is about 10%. This doping shifts the I–V plot to the lower-voltage region and increases the QE (Fig. 4).

This effect is due to reducing potential barrier (additional carriers injection) between QWs and barriers among them so j increases at a constant voltage. By varying Indium and doping concentrations in AlGaInN heterostructure active region, it is possible to increase QE and sensitivity at the same voltage.

Fig. 5 showssatisfactoryagreement between the simulation andex-perimental results and it is evident despite the fact thatthe simulation resultsare obtained withoutany additionalapproximations (abovethe basephysical models).

For comparison, it was considered the experimental current-voltage characteristics measured at the LED manufacturing company Cree Inc. for the type C460MB290E1000.

It was found that the doped barriers in the quantum-well active region of the heterostructure at $N_d = 10^{18}$ cm^{-3}, and further doping of In atomsatthe 5% levelsubstantiallyreduce the nonidealitycoefficient char-acteristics of theLEDs and increase QE. Additionally it was found that such structure shifts I-V to a lower-voltage region.

Based on simulation recommendations AlGaInN heterostructures were grown by MOCVD on SiC and Al_2O_3 substrates in the polar c-direction [0001]. Analyzing growth results (e.g. photoluminescence spectral curve and Peak lambda) it was detected that the characteristics had similar trend. The spectral mapping for heterostructure obtained by photoluminescence mapping system for peak lambda is shown in Fig. 6. Fig. 6a shows different Indium atoms concentration and distribution over wafer. Fig. 6b shows the investigation results of NH which was grown according simulation results. It can be seen the improved plane Indium atoms distribution and signal value more smooth according special doping by indium atoms.

For QE and sensitivity rise it is need to improve NH quality to more stable indium atoms distribution in QW/barriers and GaN substrates usage for reduction defects quantity. Then suggested active area structure was checked by using for photodetector.

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