Elimination of an Impact of Mechanical Stresses on an Operation of Nitride Light-Emitting Diodes

S. Morawiec, R. P. Sarzała, and W. Nakwaski
Photonics Group, Institute of Physics, Technical University of Lodz
ul. Wolczanska 219
90-924 Lodz, Poland, wlodzimierz.nakwaski@p.lodz.pl

***Abstract* –In designing of nitride light-emitting diodes, the semi-polar InAlGaN substrate is proposed to fully eliminate polarization effects.**

I. Introduction

III-N nitride materials are the most promising candidates to be used in manufacturing efficient light-emitting diodes (LEDs) in the green, blue, violet and even ultra-violet parts of the spectrum. It is well known, however, that these materials differ significantly from most of other III-V materials, which leads for example to problems with obtaining efficient sources of green radiation ("green gap" effect). Their special features mostly results from their wurtzite crystal structure, which is distinctly different from the zinc blende structure of other III-V materials. Therefore the III-N crystal unit cell is in a form of a hexagonal prism. Using the Miller-Bravais indices, its <0001> electrically polar axis is called the *c* axis and the (0001) plane perpendicular to it is called the *c* plane. Then the *a* crystalline direction is along the axis perpendicular to the *c* axis and directed towards the vertex of the hexagonal unit base. The analogous *m* axis is perpendicular to both the *c* axis and the side of the hexagonal unit base. Successive layers of most of nitride devices produced until now are manufactured along the *c* polar axis. Planes perpendicular to the *c* plane, which means – parallel to the *c* axis, are electrically non-polar. From among them, low-index $\left(11\bar{2}0\right)$ and $\left(1\bar{1}00\right)$ planes are called *a* and *m* planes, respectively. Inclined planes, i.e. planes between the polar *c* and any non-polar orientations, are called semi-polar ones, for which reduced polarization effects are expected [1].

In the ideal wurtzite structure, the *c/a* ratio should be equal to 1.633 [2], where *c* and *a* are the lattice constants in the *c* and *a* crystallographic directions, respectively. In GaN, however, this ratio is equal to 1.627, which leads to a crystal compression in the *c* direction. As a result, positive and negative charges of the Ga-N bond are shifted from each other which results in presence of electrical charges at opposite crystal surfaces. The above phenomenon is called the spontaneous polarization [2]. When additional crystal stresses are introduced (e.g. because of different lattice constants of successive structure layers), the *c/a* ratio is additionally changed, which leads to the piezoelectric polarization. In heterostructures containing quantum wells, it is followed by electrical charges at layer interfaces leading to the quantum-confined Stark effect (QCSE).

In the III-N nitrides, the spontaneous polarization is directed along the polar *c* axis of their hexagonal structure. From the very beginning of the nitride technology, there have been serious problems with appropriate good-quality and not expensive substrates. Until now most of commercially available substrates (e.g. the (0001) sapphire or (0001) SiC substrates), has the same orientation, which means that the (0001) *c* plane is usually used to manufacture nitride devices. It results in many mostly unprofitable polarization effects introduced to device volumes, the QCSE in particular. Essential progress has been made only in 2006, when *c*-oriented relatively thick GaN substrates were reported. Then, with the aid of its proper slicing, non-polar and semi-polar native GaN substrates became available.

Non-polar substrate orientation with the *c* axis parallel to the layer surface and the *a* or *m* growth planes leads to a complete elimination of spontaneous polarization. However, available high indium contents in the InGaN layer is then considerably reduced which limits possibility of generation of short-wavelength radiation. Therefore usually the semi-polar substrate orientation is used with low values of the Miller-Bravais indices, because only for them high-quality smooth growth planes may be obtained.

As it has been shown in the above text, typical nitride LEDs grown on the GaN substrate exhibit strong polarization effects. Therefore the main goal of this paper is to find such a new semi-polar InAlGaN substrate for which all these effects are eliminated. According to our anticipation, the InAlGaN material should enable polarization fitting for relatively low indium and aluminum mole fractions, easier reached technologically.

II. The Model and Results

Let us consider a typical nitride LED structure with the following layer sequence: n-type substrate, QW barrier, QW, QW barrier, electron-blocking layer, and p-type layer, all manufactured

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on a semi-polar substrate. The local co-ordinate *0xyz* system is correlated with the substrate crystalline structure (its *z* axis is directed along the *c* crystalline axis), whereas the analogous global *0x'y'z'* system has the *z*' axis at the inclination ϑ angle with respect to the *z* axis and *x*' axis along the *x* axis. At first depths of the InGaN/InAlGaN QW within the conduction and valence bands are determined assuming their ratio equal to 1.48. Polarization effects within the QW are determined with the aid of the approach similar (but not exactly the same) to the one presented in [1]. Elements of the stiffness and the polarization tensors are determined and their transformation from the local into the global co-ordinate system are carried out. Next lattice misfit parameters are calculated from the lattice constants, making possible calculations of elements of the strain tensor, which enables finding elements of the stress tensor from the tensor Hook's law. Then the spontaneous and piezoelectric polarizations are determined. which are used to compute electric fields in successive structure layers leading to determination of the band edges. The new QW band structure (modified because of the QCSE effect) enables with the aid of the Schrödinger equation determination of the energy levels, the emission wavelength and the overlapping integral between the electron and the hole wave functions.

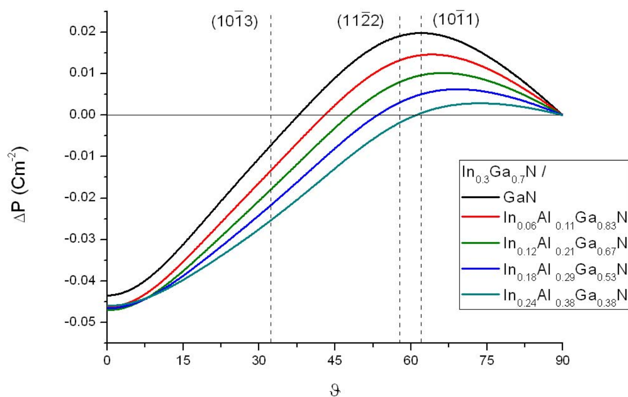

Fig. 1. Difference of the total polarization ΔP at the interface between the $In_{0.3}Ga_{0.7}N$ QW and the $In_xAl_yGa_{1-x-y}N$ barrier materials as a function of the inclination angle ϑ.

Energy difference between first energy levels of electrons and heavy holes in the $In_{0.3}Ga_{0.7}N$/GaN QW and corresponding wavelengths for the electron-hole recombination are determined as a function of the QW width without and with polarization effects included. For the desired 515-nm emission in the QW without polarization effects, the 4-nm $In_{0.3}Ga_{0.7}N$ QW has been found to be the most appropriate one. Next a possible compositions of the $In_xAl_yGa_{1-x-y}N$ barrier material adjusted with its polarization to the $In_{0.3}Ga_{0.7}N$ QW layer are analyzed. As expected (Fig. 1), the polarization difference at the QW/barrier interface is

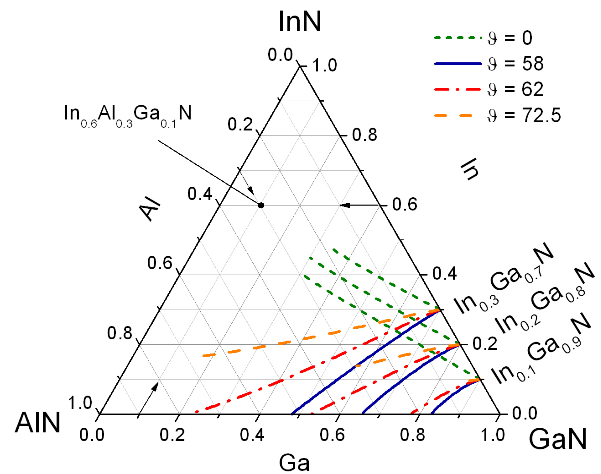

Fig. 2. Compositions of quaternary InAlGaN layers of the total polarization fitted to that of the ternary InGaN ones as a function of the inclination angle ϑ. Lines inside a triangle corresponds to three indicated compositions of the InGaN material and are plotted for four shown values of the inclination angle ϑ. Localization of the $In_{0.6}Al_{0.3}Ga_{0.1}N$ material is shown as an example (see small arrows).

equal to zero for the non-polar orientation ($\vartheta = 90^0$) but also for one semi-polar orientation. Results of more exact calculations are shown in Fig. 2, presenting compositions of InAlGaN materials of total polarizations fitted to that of the InGaN materials. As one can see, the $In_{0.19}Al_{0.20}Ga_{0.61}N$ material seems to be the most appropriate one for barriers of the $In_{0.3}Ga_{0.7}N$ QW (Fig. 2). Then, for the inclination angle of 58^0, which corresponds to the $(11\bar{2}2)$ crystallographic orientation, the potential difference between the QW and its barriers disappears. Besides its In mole fraction is still relatively low and its energy gap of only 3.1 eV leads to a reduction of the QW depth. Then the bandgap difference between the QW and its barriers is nearly the same as that in the $In_{0.2}Ga_{0.8}N$/GaN structure. Moreover, the lattice misfit between $In_{0.3}Ga_{0.7}N$ and $In_{0.19}Al_{0.20}Ga_{0.61}N$ is equal to only 1.65 %, much lower than the 2.18% determined for the $In_{0.2}Ga_{0.8}N$/GaN structure. Furthermore, the $In_{0.10}Al_{0.36}Ga_{0.54}N$ layer of the energy gap of 3.8 eV and the lattice misfit of about 3% is selected as the electron-blocking layer. For a perfect polarization fit, the QW barriers and the *p*-type layer should have the same composition as the substrate.

In conclusion, the semi-polar $In_{0.10}Al_{0.36}Ga_{0.54}N$ material used as a substrate and QW barriers in $In_{0.3}Ga_{0.7}N$ LEDs has been found to eliminate all polarization effects.

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