pyramid, and vice versa. According to the X-ray powder diffraction data (HZG-4, Ni – filter, CuK_α, diffracted beam; exposure time per frame, 15 s; scan step, 0.02°) and X-ray single crystals study (CAD-4, AgK_α, ω scan mode) there are an additional reflections related to sp. gr. *P*3. ZnO1 and ZnO2 crystals have a $[Zn(1)_{0.500}(Zn(2)_{0.475(5)\ 0.025})]Zn_{0.015(5)(i)}[(O(1)_{0.490(6)\ 0.010})O(2)_{0.500})$ and $[(Zn(1)_{0.465(6)\ 0.035})Zn(2)_{0.500}]Zn_{0.035(6)(i)}(O(1)_{0.500})(O(2)_{0.500})$ refined compositions, respectively. The compositions are in good agreement with the results of X-ray microanalysis (INCA Penta FETx 3). Zinc and oxygen atoms occupy two positions Zn(1), Zn(2) and O(1), O(2) both completely, and partially. Besides, the presence of different quantity of interstitials atoms – Zn_i in the structures of ZnO1 и ZnO2 was found. The alternation of full filled and partially filled Zn and O «layers» in the ZnO structure leads to a symmetry decrease in the local area of the crystal (from sp. gr. $P6_3mc$ to sp. gr. *P*3).

Due to the fact that X-ray microanalysis did not reveal the presence of impurity atoms and the compositions of green and light green samples differ only in the oxygen content, it can be assumed that the color of ZnO crystals is associated with the oxygen vacancies content: a decrease of oxygen vacancies leads to discoloration of the ZnO crystals. In transmission spectra («Specord-M40») of ZnO two bands are observed: ~445 μm (ZnO1 and ZnO2) и ~625 μm (ZnO1) which correspond to oxygen vacancies - $V_O^{\bullet n}$ and color of the crystals, respectively. The color of crystals can be ascribed to a $(V_O^{\bullet n}, ne')^x$ associate formation, namely centre coloration.

The relationship between the oxygen vacancies content and the structural perfection (diffractometer D8Discover: $CuK_{\alpha 1}$; Ge (002)) of the crystals has been found: the light-green sample is characterized by the lower values of the half-width of the Bragg peak 0002 (28.8'' for ZnO1 with $(Zn_{0.975\ 0.025})Zn_{i(0.015)}(O_{0.990\ 0.010})$ general composition and 22.4'' for ZnO2 with $(Zn_{0.965\ 0.035})Zn_{i(0.035)}O$ one). Moreover, the resistivity (ρ) and activation energy (E_a) are higher for the light-green sample (ρ =1.5(1)·10^8 Om·cm, E_a=0.51(9) eV) than that for the green sample (ρ =1.6(1)·10^7 Om·cm, E_a=0.38(9) eV).

Keywords: X-ray_study, defects, color

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Defect determination in epitaxial a-plane GaN Layers_

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The technological application of (0001), i.e., c-oriented GaN is complicated by the piezoelectric effect along the [0001] direction and non-polar GaN thin films overcome this problem. However, this type of material possesses a large number of defects, especially stacking faults (SF) so that a reliable method for the determination of the defect densities is therefore of large importance.

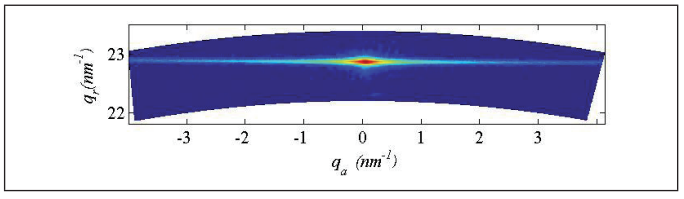

Fig.1. Example of the reciprocal space map of x-ray diffuse scattering measured in the symmetric non-coplanar 10-10 diffraction from an a-GaN epitaxial layer. The axis q_a and q_r are parallel to the sample surface and to the (inclined) diffraction vector, respectively.

We investigated non-polar a-plane oriented GaN epitaxial layers with the (11-20) surface orientation. In these layers, two types of SFs occur with the displacement vectors R = 1/6(20-23) and 1/3(1-100). If g.R ≠ n (g is the diffraction vector, n is an integer), the diffuse x-ray scattering from the SFs has the form of [0001]-oriented streaks [1] perpendicular to the fault planes. We have measured the streaks in symmetric non-coplanar diffractions 10-10, 20-20 and 30-30, using a high-resolution x-ray diffraction setup in a series of a-GaN epitaxial layers with various densities of stacking faults (Fig. 1).

We compared the measured intensity distributions along the streaks with simulations supposing a random Markov-like sequence of stacking faults and kinematical approximation; from the comparison we determined the prevailing displacement vector ***R*** of the SFs and the fault density.

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Keywords: Diffraction, Gallium, Nitride.

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High resolution x-ray diffraction analysis of AlGaSb/GaSb

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GaSb single crystals are the ideal substrates for the growth of InGaAsSb, AlGaAsSb, AlGaAs and AlGaSb heterostructures to fabricate optoelectronic devices. GaSb surfaces are highly reactive to oxidation, the oxides grown on their surface have poor conductivity (~10^{-2} Ω^{-1} cm^{-1}) and it produces high surface leak currents. Using the liquid phase epitaxy (LPE) technique under supercooling conditions we have grown $Al_xGa_{1-x}Sb$ layers doped with tellurium to (100) on n-GaSb(with $0.05 \leq x \leq 0.2$). Using Raman spectroscopy we characterized the structural quality. The Raman spectra show two main peaks located about 224 and 234 cm^{-1}, which were deconvoluted by four Lorentzians. In order to assign the peaks use is made of the random-element isodisplacement (REI) model. Comparison of the experimental results with the values obtained by REI model allows us to confirm that the bands correspond to the LO-like and TO-like of the binary compounds, GaSb. High-resolution X-ray diffraction (HRXRD) has been used to characterize these structures. The out of plane lattice parameter, was estimated directly from the symmetrical diffraction for (001) alloys. These results show that all the layers are relaxed.

Liquid phase epitaxy (LPE) growth was carried out in a single-zone isothermal furnace in hydrogen using the horizontal sliding boat technique. The boat was made from high purity graphite, $Al_xGa_{1-x}Sb$, were grown nominally lattice-matched to vicinal (100) n-GaSb substrate at a temperature of 673 K. Raman scattering experiments were performed at room temperature using 6328 Å line of a He-Ne laser at normal incidence for excitation. The nominal laser power used in these measurements was 20 mW. Structural characterization of the samples is carried out by means of HRXRD in a Bruker D8 Discover diffractometer, parallel beam geometry and monochromator of gobel mirror, CuKα radiation, 1.5406 Å operated at 40kV and 40mW, in the range of 20° <2θ <80° by step of 0.02°.

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