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NON-STOCHIOMETRY AND X-RAY ANALYSIS OF ZnSe/ZnO:O NANOGETEROSTRUCTURES AND ZnSe/ZnO:O,Zn NANOHETEROJUNCTION

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ABSTRACT: *The crystal structure, size, shape and orientation of ZnO nanoparticles were determined depending on the Zn/Se ratio and O and Zn_i impurities in ZnSe/ZnO:O nanoheterostructures and ZnSe/ZnO:O,Zn nanoheterojunctions. It was shown that these structures had nonstoichiometry of the ZnSe surface layer (0.85–0.86) and the size of ZnO nanocrystallites with the orientation: film (103)ZnO ~ 27 nm on the (311)ZnSe face.*

Keywords: nanogeterostructures, nanoheterojunction, ZnSe/ZnO:O,Zn, ZnO, nanoparticle, , X-ray diffraction and phase analysis, reflection, nonstoichiometry, nanometr.

In the republic, much attention is paid to the development of fundamental principles for the manufacture of various types of semiconductor nanoheterostructures and nanorods for the creation of optical radiation detectors - photodiodes, phototransistors and photothyristors, infrared converters - radiation to visible, optoelectronic devices - heterolasers at the world level [1-3]. As result of these studies, it was shown that heat treatment in Zn vapor of ZnSe single crystals improves the electrical and optical properties due to the formation of Zn_i centers and stable associates ($O_{se}V_{Zn}Me^{III}_{Zn}Zn_i$) [3]; ZnO/ZnSe hetero-nanocoils for use as photodetectors and light-emitting diodes were obtained; type II n-ZnO/p-ZnSe heterostructure for photodetectors.

However, no connection was made between radiolysis and nonstoichiometry, the possibility of creating ZnO/ZnSe:O,Zn nanoheterojunctions.

The aim of the study was to determine the crystal structure, size, shape and orientation of ZnO nanoparticles depending on the Zn/Se ratio and O and Zn_i impurities.

The object of the study is ZnSe scintillator crystals, heat treated in zinc vapor and an oxidizing medium [3].

Research methods. X-ray fluorescence analysis was carried out on a multichannel analyzer with a Ge-detector in order to determine the total elemental composition averaged over the surface layer by selecting radioactive sources of X-ray excitation of k-lines of elements to the depth of the half-absorption layer. To determine the degree of nonstoichiometry of a crystal, i.e. the Se/Zn ratio in the near-surface layer was about 40 μm, the ^{109}Cd isotope with an X-ray energy of 22.1 keV was used, and the ^{241}Am isotope with an X-ray energy of 59.6 keV was used to find the concentration of the Te impurity in the 70 μm layer, the error was no more than 0.1%.

The structure and phase composition of the samples were investigated by small-angle X-ray diffraction on a DRON-3M diffractometer (radiation $\lambda_{CuK\alpha}$=0.1542 nm) in the range of angles $2\Theta=10\div70^0$. Analysis of the obtained X-ray diffraction patterns makes it possible to determine the symmetry of the crystal structure, the crystallographic plane of the sample surface, and the general phase composition [4]. The collimation of an X-ray beam and the use of the small-angle scattering method make it possible to identify both amorphous regions and crystalline inclusions, and to determine their sizes on a nanometer scale using the well-known Selyakov-Scherrer formula.

$$L = \frac{0.94\lambda}{\beta_{hkl} \cdot Cos\theta_{hkl}}$$

where L - is the grain size (nm), λ - is the wavelength of the radiation used, θ is the angle of reflection, β - is the half-width of the corresponding reflection, in rad. The error in determining the size of ZnO nanoparticles was no more than ± 1%.

Crystal structure: Thermal neutron diffraction in $Zn_{1-x}Ni_xSe$ (x=0.0025), $Zn_{1-x}Cr_xSe$ (x=0.0029), $Zn_{1-x}V_x^{2-}Se$ (x=0.0018), $Zn_{1-x}Cr_x^{2-}Se$ (x=0.0006), $Zn_{1-x}Ni_xO$, as well as trigonal ZnSe:Ni, ZnSe:V and tetragonal ZnSe:Cr semiconductors, the existence of a phase

transition, structural distortions of the lattice, diffuse scattering concentrated in the vicinity of strong Bragg reflections, caused by nanoscale shear deformations of the ZnSe lattice, the types of which are determined by the Jahn – Teller effect by 3d ions, have been revealed [5]. In X-ray diffraction patterns of ZnSe, peaks (111), (220) (311) and (400) were observed in the region from $2\theta=10\div75^0$ [6]. The self-ordering of isoelectronic Mg and O impurities in ZnSe is described theoretically; it is shown that the advantage in the formation of Mg-O and Zn-Se bonds over the formation of Mg-Se and Zn-O bonds leads to self-organization of Mg and O impurities in ZnSe in a wide concentration range [7].

Crystal structure and phase composition

XRF table using an isotope source and a Si (Li) detector

ZnSe:O и ZnSe:O,Zn			
Weight, gr	Conc. Zn, масс %	Conc. Se, масс %	Rel. Se/Zn
0.3586 - 0.3612	33.71 - 33.86	28.48 - 28.68	0.845 - 0.847

It can be seen from the table that the ZnSe/ZnO:O NGS in the near-surface layer were nonstoichiometric and contained 1 wt% excess Zn. The super-stoichiometry of Zn, due to the volatility of Se, increases after HT in Zn vapors, due to the difference in the bonding forces of Zn-Se and Zn-O, the activation energy of diffusion of Zn into interstices, and the energy of formation V_{Se}.

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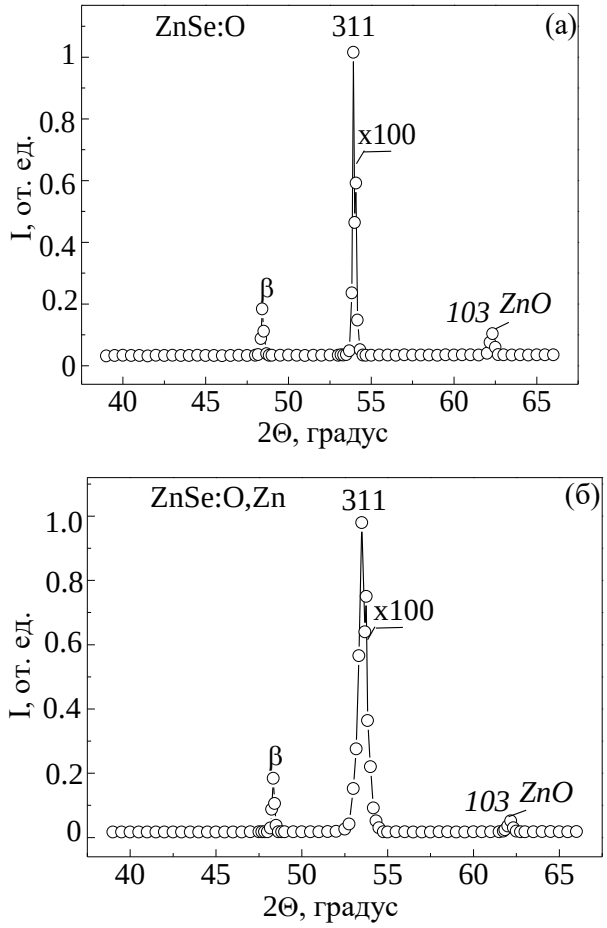

Figure - X-ray phase analysis of ZnSe:O before (a) and after (b) heat treatment in Zn vapor. The real intensity (311) is 100 times greater.

The figure shows the results of X-ray phase analysis (XRD) of ZnSe:O crystals before and after HT in Zn vapor. The ZnSe:O crystals were cut parallel to the close-packed plane (111); accordingly, the X-ray diffraction pattern shows the most intense basal reflection (311). It can be seen that low-symmetry impurity ZnO phase (reflection 103) and a very monotonic background are observed in an untreated cubic ZnSe crystal. This suggests that the ZnSe matrix lattice has relaxed and is no longer stressed. Intensity ratio I(103)/I(311) ~ 0.0091 (left). Hence, it follows that the initial ZnSe: O crystal is apparently a structure in the surface layer of which ZnO NC were formed.

After HT in Zn vapor, the matrix reflection (311) noticeably broadened and the splitting along α_1-α_2 weakened, and the content of the ZnO impurity phase, estimated from the intensity ratio I(103)/I(311)~0.0086 (right), slightly decreased. The observed broadening of

the (311) reflection of the matrix lattice can be attributed to elastic stresses upon diffusion doping with Zn atoms occupying interstitial positions.

As indicated above by XRD, that the samples under study were nonstoichiometric: 49 wt. Se% to Zn mass 51%, which means $3.75 \cdot 10^{21}$ cm^{-3} Se atoms to Zn atom $4.68 \cdot 10^{21}$ cm^{-3}. In this case, the excess of Zn_i atoms (or the number of VSe) was $\sim 0.9 \cdot 10^{21}$ $см^{-3}$ [8]. The presence of an energy level in E_g associated with Zni is confirmed by optical and electrical measurements. The sizes of inclusions of the crystalline phase of ZnO, determined by the Selyakov - Scherrer formula, were ~ 27 nm. The size of the ZnO film, also estimated using the Scherrer formula, was [9] 18 nm. In the X-ray diffraction patterns of ZnSe, peaks (311) were observed in the region from $2\theta=10\div75^0$ [10], and for ZnO 100, 002, 101, 102, 110, 103, 112, 201, 004 at $2\theta=32\div72^0$ [11].

In our case, X-ray diffraction analysis showed that, depending on the composition and orientation of the crystals, the ZnSe matrix lattice gave the (311) reflection in the region $2\theta=52\div55^0$, and the NC ZnO gave the (103) reflection at $47\div49^0$. In the same place, estimates are given of the maximum average transverse size of NP in the range from 40 to 50 [9] and 20–40 nm had discrete levels in the conduction band depending on the E_g of the material. In our case, the critical size of ZnO NP in NGS and NHJ was 27 nm. Thus, the results obtained by us on X-ray structural analysis are consistent with the data of works published later [9-11].

CONCLUSION: For the first time, direct correlation between the nonstoichiometry of the ZnSe surface layer (0.85-0.86) and the size of the formed ZnO nanocrystallites with the orientation: film (103) ZnO ~ 27 nm on the (311) face of the ZnSe/ZnO:O NGS and ZnSe/ZnO:Zn NHJ

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