pyramid, and vice versa. According to the X-ray powder diffraction data (H2G-4, Ni – filter, CuKα, diffracted beam; exposure time per frame, 15 s; scan step, 0.02°) X-ray single crystals study (CAD-4, AgKα, 0 scan mode) there are an additional reflections related to sp. gr. P3. ZnO1 and ZnO2 crystals have a [Zn(1),0.500(Zn(2),0.465 0.023)]Zn(0.135,0.062)(O(1),0.265,0.000)O(2),0.000 and [(Zn(1),0.500 0.023)Zn(2), 0.465]Zn(0.135,0.062)(O(1),0.265,0.000)O(2),0.000 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 – Zni in the structures of ZnO1 n ZnO2 was found. The fullness of 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. P63mc to sp. gr. P3).

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 (αSpectord-M40b) of ZnO two bands are observed: ~445 µm (ZnO1 and ZnO2) and ~625 µm (ZnO1) which correspond to oxygen vacancies – V不可避免, and color of the crystals, respectively. The color of crystals can be ascribed to a (V不可避免,不可避免) associate formation, namely centre colouration.

The relationship between the oxygen vacancies content and the structural perfection (dифферентометр D8Discover: CuKα; 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(0.75,0.025)Zn(0.25,0.000)O(0.990,0.010)O general composition and 22.4° for ZnO2 with (Zn(0.990,0.010)Zn(0.010,0.000)O one). Moreover, the resistivity (ρ) and activation energy (Ei) are higher for the light-green sample (ρ =1.51)·10Ω·cm, Ei =0.51(9) eV) than that for the green sample (ρ =1.6(1)·10Ω·cm, Ei =0.38(9) eV).

Keywords: X-ray study, defects, color

**MS28.P07**

Defect determination in epitaxial a-plane GaN Layers.

Mykhailo Baruchuk,1 Václav Holý,2 Sergei Layarev,3 Sondes Bauer,3 Charles University in Prague, (Czech Republic). 3Karlsruhe Institute of Technology, (Germany). E-mail: mikebarchuk@rambler.ru

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.

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 ≠ 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.


Keywords: Diffraction, Gallium, Nitride.

**MS28.P08**

High resolution x-ray diffraction analysis of AlGaSb/GaSb

Arturo Méndez-López,1 Jorge Contreras-Rasco,1 Joel Diaz-Reyes,2 Javier Martinez-Juarez,3 Miguel Galvan-Arellano,3 “Semiconductor Devices, Benemérita Universidad Autónoma de Puebla, Puebla, (México). 2Center for Research in Applied Biotechnology, Instituto Politecnico Nacional, Tlaxcala, (México). 3Research and Advanced Studies Center, Instituto Politecnico Nacional,Distrito Federal, (México). E-mail: art1396@gmail.com

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 (~10Ω·cm) and it produces high surface leak currents. Using the liquid phase epitaxy (LPE) technique under supercooking conditions we have grown Al1-xGa_xSb layers doped with tellurium to (100) on n-GaSb with 0.05 ≤ x ≤ 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, Al1-xGa_xSb, 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 gøbel mirror, CuKα radiation, 1.5406 Å operated at 40kV and 40mW, in the range of 20° <2θ <80° by step of 0.02°.


**Keywords:** X-ray, raman, epitaxy

**MS28.P09**

*Acta Cryst. (2011) A67, C408*

**Growth and characterization of p-type ZnO films byArsenic thermal diffusion**


ZnO can be used as a UV light emitter and ZnO could be used to excite phosphors to produce white light. ZnO p-n junctions were reported with phosphorus doping [1]. However, it is needed to develop new and easily p-doping methods for formation of p-n junctions in ZnO. We reported a simple and novel homemade system to obtained ZnO p-type.

ZnO n-type single crystal substrates were obtained from MTI Corporation. The Arsenic doping was introducing through arsenic diffusion. p-n junctions have been formed in single-crystal ZnO substrates by diffusion of As. The properties of ZnO:As films were studied by x-ray diffraction (XRD), X-ray spectroscopy (XPS), Raman scattering and photoluminescence (PL) measurements. Hall-effect measurements were done at room temperature. A decrease on carrier concentration, mobility and resistivity were obtained. The decrease on the electrical values is related to self compensation between native defects and arsenic interstitials. ZnO p-type thin film layer was obtained by simple method with As diffusion on ZnO single crystal.


**Keywords:** ZnO, p-n homojunctions, As diffusions

**MS28.P10**

*Acta Cryst. (2011) A67, C408*

**Physical properties of ZnS thin films grown on GaAs by RF magnetron sputtering**

Eladio Flores-Mena,1 Joel Díaz-Reyes,a Javier Martinez-Juárez,a Arturo Méndez-López,b Moisés Gutiérrez-Arias,a Monserrat Morín-Castillo,b Miguel Galván-Arellano,a Facultad de Ciencias de la Electrónica, BUAP, Puebla, Puebla (México).b Centro de Investigación en Biotecnologia Aplicada,IPN, Tepetitla, Tlaxcala (México).cCentro de Investigaciones en Dispositivos Semiconductores, BUAP, Puebla, Puebla. (México).dDepto. Ing. Eléctrica, SEES, CINVESTAV-IPN, México, D.F. (México). E-mail: eflores@ece.buap.mx

As one of the most important II-VI group semiconductors, zinc sulfide (ZnS) with a wide direct band gap of 3.8 eV has been extensively investigated and used in electroluminescent devices, flat panel displays, infrared windows, sensors, and lasers. To explore the possibility of using it in electroluminescent devices, a study of the structural and optical properties of the host material is an important step. Based on the above criterion, the structural and optical properties of ZnS films have been studied in the present work. ZnS thin films were grown on GaAs (001) substrates at different temperatures by RF magnetron sputtering. The XRD analysis reveals that deposited films below 335 °C, assumed the zinc blend structure. Samples annealed at temperature above 335 °C showed mixed phases of the zinc blend and wurzite structures. Information about crystallite size is obtained from (001), (111) and (104) diffraction peaks. The average crystallite size of the film was determined to be w 32 nm using the Scherrer formula. Besides it made a experimental and theoretical study on first- and second-order Raman scattering of zinc blend. Based on the calculated phonon band structure, phonon density of states, and symmetry selection rules, one has clearly identified for the first time the origins of these vibration modes in the second-order Raman spectra.

**Keywords:** II-VII, X-ray, sputtering

**MS28.P11**

*Acta Cryst. (2011) A67, C408*

**Growth of transition metal doped AIN single crystal and its stimulated emission**

Wenqiong Wang, Liangbao Jiang, Sibin Zuo, Shunchong Wang, Hui Li, Kaixing Zhu, Jun Wang, Xiaolong Chen Research and Development Center for Functional Crystals, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O.Box 603, Beijing 100190, (China). E-mail: wjwang@iphy.ac.cn

Aluminum nitride (AlN) as a wide band gap semiconductor has attracted increasing attention. Transition metals (TM) doped AlN micro/nano structures also have gained increasing attention for its potential applications in the field of optical and spintronic devices. However, most of the researches are focused on the influence of TM on the magnetism and photoluminescence properties of AlN micro/nano structures. In this work, we report the observation of the stimulated emission of TM doped AlN crystalline whisker.

Transition metal (Fe, Ni) doped AlN crystalline whiskers were grown by PVT method in a RF-heated furnace. Graphite crucible with 32mm in inner-diameter was used as heating element. TaC crucible with 30mm in inner-diameter and 50mm in depth was placed in the graphite crucible as AlN charge container. Under typical growth conditions, the reactor pressure was 0.6atm and the source temperature was maintained at 1700°C. AlN (99.99%) and Fe or Ni (99.99%) powders were used as reacted sources. The doping concentration of TM was controlled by the mole ratio of TM in the source material. Large scale triangular AlN whiskers were successfully grown. We found that TM has the function to control the morphology of the AlN whisker. The doped AlN whiskers show triangular shape while the undoped AlN whiskers were hexagonal shape. The optical characteristics of the doped AlN whiskers were investigated. Stimulated emission at about 607 nm with the linewidth less than 0.2 nm from single Fe-doped AlN triangular whisker was firstly demonstrated at room temperature. Longer luminescence lifetime of over 2.5ms was observed. Our work demonstrates that AlN single crystal is a new excellent host for solid state laser which might open a door to new high power lasers.

**Acknowledgment:** This work is supported by The National Basic Research Program of China (973 Program) grant No. 2007CB936300, the National High Technology Research and Development Program of China (863 Program) grant No. 2006AA03A107 and the National Natural Science Foundation of China (grant No. 50702073).

**Keywords:** AlN, single crystal growth, growth from vapor