**PS10.07.13 $Er^{3+}$-DOPED $KTiOPO_4$ WAVEGUIDE BY ION EXCHANGE.** P.Q Huang and P.A. Thomas, Department of Physics, University of Warwick, Coventry CV4 7AL, U.K

Optical waveguides of $Er^{3+}$-doped $KTiOPO_4$ were formed, for the first time, using an ion exchange process. Scanning electron microscopy and secondary ion mass spectroscopy have been used to study the depth distribution of the $Er^{3+}$ ions and the morphology of the erbium doped crystal. The diffusion concentration was found to change two orders of magnitude in a depth of 8μm. There was no obvious diffusion of $Er^{3+}$ ion into $KTiOPO_4$ in the temperature range of 400-600°C. The erbium concentration and depth were improved after annealing at 800°C for a few minutes to four hours in crystals. Strong characteristic $Er^{3+}$ intra-4f shell emission 1500-1600nm $^4I_{13/2}$ - $^4I_{15/2}$ was observed at 295K. Fluorescence showed a 2~6nm lifetime and was site-dependent. The polarization dependence of the emission spectra at 1508nm suggested that the KTP crystal structure was preserved in the doped layer. The experimental results obtained so far have shown a promising outlook for the development of a waveguide laser and an amplifier based on $Er^{3+}$-doped KTP.

**PS10.07.14 STRUCTURE AND PROPERTIES OF $Na_{0.17}K_{0.83}TiOPO_4$ SINGLE CRYSTAL, SYNTHESIZED BY FLUX METHOD** D.Y.Lee, N.I.Sorokina, I.A.Verin, V.I.Simonov, Inst.of Crystallography RAS, Leninskii pr.59, Moscow, 117333, Russia, V.I.Voronkova, V.K.Yanovsky, Moscow State U.,Dept. of Physics, Leninskiye Gory, Moscow, 117234, Russia.

Structure of $Na_{0.17}K_{0.83}TiOPO_4$, which belongs to the crystal type of $KTiOPO_4$ characterized by nonlinear optical properties and superionic conductivity, was analyzed by single crystal X-ray diffraction method and the structure-property correlation of this crystal was investigated. A single crystal, used for experiment, was prepared by spontaneous crystallization from flux. The temperature dependence of relative dielectric constant E33 and electric conductivity of crystals S33 were measured at a frequency of 1MHz by means of the TESLA BM341E bridge. A full X-ray structural study was performed on CAD-4F ENRAF-NONIUS autodiffractometer, using MoK radiation. The structure was refined, using Prometheus program. A special attention was given to cation sites, occupied by $K^+$ and $Na^+$ in the channels in firm $TiO_6$ framework. At these sites anharmonic thermal motion was established and thermal parameters were calculated up to 4th order tensor. In the difference Fourier map an additional peak of about 1 e/Å$^3$ was found around the $(K, Na)_2$ site and through the analysis of this peak the structure was better refined. It was reported that in the crystals of $Na_xK_{1-x}TiOPO_4$ type the reducing of nonlinear optical properties took placed with the replacement of K by Na, although the structure was almost the same. The reason of this phenomenon is, however, not clear enough. That is why an accurate structural study of this crystal is so important in establishing the structure-property correlation and comparing with those of $KTiOPO_4$ and $NaTiOPO_4$.

**PS10.07.15 POLYMORPHISM AND CO-CRYSTALS:A CASE STUDY OF AMINO-NITROPYRIDINES.** By M.Nieuwenhuyzen and C.B.Aakeroy.

The crystal structures of four compounds from a family of commonly used building blocks for non-linear optical materials, amino-nitropyridines, have been determined, 2-amino-5-nitropyridine[1] **1**,the solvated compound 2-amino-5nitropyridine monohydrate[1] **2**, a new polymorph of 2-amino-3-nitropyridine[1] **3**, and the co-crystal 2-amino3-nitropyridine with 2-amino-5-nitropyrimidine[2] **4**. These compounds are all stabilised by a combination of hydrogen bonds (including C—H .... X interactions) and ring-ring interactions. The balance between these intermolecular forces and the way they influence the packing of these materials is examined, and the problems associated with polymorphism in this system is addressed.

*References:*
1) C.B.Aakeroy, M.Nieuwenhuyzen, A structural study of 2-amino-5nitropyridine and 2-amino-5-ntropyridine; Molecular building blocks for non-linear optical materials., submitted to *J. Mat. chem.*.
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**PS10.07.16 CRYSTAL STRUCTURE OF VACANCY ORDERED $ZnGa_2Se_4$.** O. Nittono, T. Hanada, and Y. Nakamura, Department Metallurgical Engineering, Tokyo Institute of Technology, Oh-Okayama, Meguro-ku Tokyo 152, Japan

$ZnGa_2Se_4$ is a representative of II-III-VI compound semiconductors and the basic structure is chalcopyrite. In the $ZnGa_2Se_4$ compound, Se sublattice is perfect fcc but the cation sublattice is ternary: Zn, Ga and structure vacancy. The structure of $ZnGa_2Se_4$ is reported to be either defect stannite or defect chalcopyrite whose space group is I 2m or I respectively. In each structure, metal atoms and the structure vacancy are arranged in order. They are different in the configuration of metal atoms and structure vacancy even though the projected structures on the fundamental planes are identical. In the present work, convergent electron beam diffraction (CBED) are applied to determine the space group of $ZnGa_2Se_4$, and then crystal structure is refined by X-ray Rietveld method.

The specimens of $ZnGa_2Se_4$ are synthesized by melting of $Ga_2Se_3$ (3N) and ZnSe (5N) at 1673K, and then annealed at 1273K for 60 days. Sharp reflection spots are observed in the selected area electron beam diffraction (SAED) patterns, which indicates the good crystallinity of the specimens. TEM observation shows that domains grow up well and the size is as large as 5μm. A CBED whole pattern taken along the [001] direction clearly exhibits $4_Rmm_R$ symmetry, so that it is found that $ZnGa_2Se_4$ belongs to the space group I m2. Based on the result, X-ray Rietveld refinement (F. Izumi, 1993) has been done and that converged at a=5.5093Å, b=10.9450Å, $R_{wp}$=18.49%, $R_F$=5.60%, S=1.7065.

F. Izumi, "The Rietveld Method," ed. by R. A. Young, Oxford University Press, Oxford (1993), Chap. 13

**PS10.07.17 NEW-TYPE INTERFERENCE PATTERN GENERATED BY INTERNAL STRESS AROUND A MICROPIPE IN THE 6H-SiC SINGLE CRYSTAL.** By H. Ohsato[1], T. Kato[1], M. Razeghi[2], T. Okuda[1], [1]Department of Materials Science and Engineering, Nagoya Institute of Technology, Nagoya 466, Japan, [2]Center for Quantum Devices, Northwestern University, IL 60208-3118, USA

SiC has been expected for substrate for GaN single crystal thin film which is available for blue laser diode, but the crystalline quality of SiC substrates is low grade affected by internal stress around micropipes. Usually, sapphire ($\alpha$-$Al_2O_3$) is the most commonly used for substrates, as it gives the best crystalline quality. Moreover GaN grown on sapphire has been used for blue LED and emission of blue laser has just succeeded. But there are many defects on the interface which cause short lifetime because of large atomic distance mismatch (ADM) between GaN and sapphire. On the other hand, good quality GaN epilayer has not grown on the SiC substrates in spite of small ADM. SiC single crystals made by modified Lely's method which could grow large single crystals have many micropipes along *c*-axis. Butterflytype strain configurations around micropipes have been observed by the orthoscope under optical polarizing microscope in spite of adjusting *c*-axis direction to the optical axis of the microscope using universal stage. The butterfly-type pattern has been settled as a new-type interference pattern. A forth working upon the micropipe to one direction has been appreciated from the interference pattern with vibration directions (Fig.1). The vibration directions of the fast and slow wave are corresponding to the direction of composition and tension, respectively. Clarification of the growth mechanism of micropipes accompanied internal stress is available for growth of good quality GaN.

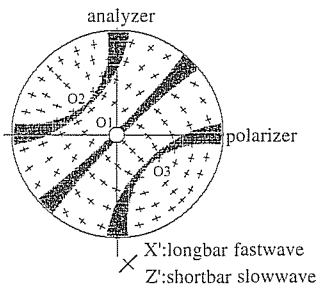


Fig.1. O1:micropipe, O2& O3: no birefringence points