compound Li<sub>3.17</sub>(P<sub>0.69</sub>Ge<sub>0.24</sub>Mo<sub>0.07</sub>)O<sub>4</sub> has been grown on Pt-rod. For the structure determination there was chosen the single crystal with size 0.13x0.17x0.20 mm.

Crystal structure of analyzed compound is similar to the structure of  $Li_{3+x}P_{1-x}Ge_xO_4$  (x=0.31). The partial substitution of  $Ge^{4+}(P^{5+})$  for Mo<sup>6+</sup> follows with the decrease of Li-atom content. In spite of it a significant amount of Li occupy 3 additional sites - 2 tetragonal (very close to 2 main Li-positions which are partially vacant) and 1 octahedral. The fourth additional Li-site found in  $Li_{3+x}P_{1-x}Ge_xO_4$ (x=0.31) in our compound is empty.

This work was supported in part by the Russian Federation President Grant for supporting the leading scientific school NSh-1954.2003.2. The authors thank Prof. E. Tillmanns and Dr. U. Kolitsch for their help in data collection.

Keywords: crystal growth, conductors, electrocrystallization

### P.16.04.2

Acta Cryst. (2005). A61, C441

Phenomenon of Polytypism in Melt Grown Layered Crystals of CdI<sub>2</sub>, PbI<sub>2</sub>.and CdBr<sub>2</sub>

Sunil Kumar Chaudhary, Harjeet Kaur, University college, M.D. INDIA University, Rohtak-124001, E-mail: Sunilkc2001in@yahoo.com

Polytypism has been observed in a large number of materials where the nearest neighbor relationship between identical twodimensional layers of atoms can be satisfied in more than one way . The phenomenon has posed interesting problem for the Scientists, since the nature of force that causes ordering over the scale ranging from few angstrom to few thousands of angstrom units is not known.

The theoretical and experimental advancements made in the study of polytypism in melt- grown crystals of CdI<sub>2</sub>, PbI<sub>2</sub> and CdBr<sub>2</sub> in the last few decades have been reviewed. The past work done in this field by us (using optical, Lasers and X-ray diffraction techniques) and update on the aspect of polytypism in the above crystals has been outlined with special reference to the role of:

(1) Purification and effect of impurities (known and unknown);

(2) Solid state phase transitions in the above crystals;

(3) Temperature dependence and their thermodynamic stability. Keywords: polytypism, X-ray diffraction, melt growth

## P.16.04.3

Acta Cryst. (2005). A61, C441

## Nonstationary Heat field as a new Approach in Bridgman Crystal Growth

Konstantin Kokh<sup>a</sup>, Alexander Kokh<sup>b</sup>, Gennady Shvedenkov<sup>a</sup>, <sup>a</sup>Novosibirsk State University. <sup>b</sup>Branch of the Institute of Mineralogy and Petrography, Russia. E-mail: kostya@demakova.net

A traditional and axiomatic approach in crystal growth is the creation of a stable and stationary heat field with desired axial and radial temperature gradients. However, an obvious progress in application of Heat Field Rotation Method [1] is reached by development of the non-linear crystal growth technologies of β-BaB<sub>2</sub>O<sub>4</sub> (BBO) in Czochralski configuration, LiB<sub>3</sub>O<sub>5</sub> (LBO) and CsLiB<sub>6</sub>O<sub>10</sub> (CLBO) in Kyropulos method.

The experiments of AgGaS<sub>2</sub> crystal growth by Bridgman method were performed using modified furnace which allows to create cyclic temperature oscillations. Obtained results suggests that moderate temperature oscillations (up to 4°C) favor the crystal quality and are likely to affect generally the hydrodynamic situation in the melt according to Curie principle. More complete mixing resulted to the crystals free of crack, twins and inclusions. Such defects often accompany crystals grown in stationary heat field where the mixing generated by natural convection is slowed due to "stabilized" axial temperature distribution in the melt.

[1] Kokh A.E., Popov V.N., Mokrushnikov P.W., J. Crystal Growth, 2001, 230, 1-2, 163.

Keywords: crystal growth apparatus design, convection, nonlinear optical materials

# P.16.04.4

Acta Cryst. (2005). A61, C441

Growth and Crystal Structure of Bismuth Octaborate, α-Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub> Fedor Yu. Zavartsev<sup>a</sup>, G. M. Kuz'micheva<sup>b</sup>, V. B. Rybakov<sup>c</sup>, S. A. Koutovoi<sup>a</sup>, I. A. Shcherbakov<sup>a</sup>, A. I. Zagumennyi<sup>a</sup>, <sup>a</sup>General Physics Institute of RAS. <sup>b</sup>Moscow State Academy of Fine Chemical Technology, <sup>c</sup>Moscow State University. E-mail: fzavart@lsk.gpi.ru

The objects of this search were a study of Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub> crystallization in the melts of near stoichiometric compositions, a determination of bismuth octaborate solid solutions range and a refinement of crystal structure of low-temperature phase of bismuth octaborate,  $\alpha$ -Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub>.

The bismuth octaborate crystals were grown from the melts of stoichiometric (20mole% Bi2O3 /80 mole% B2O3) and near stoichiometric (21.9mole% Bi2O3 / 78.1mole% B2O3) compositions. The grown crystals of a plate like form were of (5-7) mm in thickness, 27 x 27 mm<sup>2</sup> in cross-section. Comparison of lattice parameters of  $\alpha$ -Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub> crystals (a=4.3191(9), b=22.175(7), grown c=6.4739(19)Å,  $\beta$ =105.44(2)°, sp.gr. P2<sub>1</sub>, z=2) with the data presented in [1, 2] indicates that the phase of non-stoichiometric, Bi<sub>2</sub>O<sub>3</sub>-rich, composition exists unlike to the  $\alpha$ -Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub> phase studied by authors of [1, 2]. Structure was refined as a racemic twin with components 0.80 and 0.20. Range of solid solutions having the 78.1mol.%  $B_2O_3$  – 84.7mol.% B<sub>2</sub>O<sub>3</sub> boundaries exists for the Bi<sub>2</sub>O<sub>3</sub>·4B<sub>2</sub>O<sub>3</sub> compound.

[1] Teng B., Yu W. T., Wang J. Y., Cheng W. F., Dong S. M., Liu Y. G., Acta Cryst, 2002, C58, i25. [2] Egoryusheva A.V., Kanisheva A.S., Kargin Yu. F., Gorbuova Yu. E., Mikchailov Yu. N., Journ. Inorganic Chemistry, 2002, 47. 1961.

Keywords: bismuth octaborate, crystalline solid solutions, crystal structure

# P.16.04.5

Acta Cryst. (2005). A61, C441

Flux Growth and Characterization of Gallium-substituted YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> Crystals

Victor Maltsev, Nikolay Leonyuk, Department of Crystallograph Geological Faculty, Lomonosov Moscow State University. E-mail: maltsev@geol.msu.ru

Non-centrosymmetric YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> (YAB) crystals of huntite structure, especially, doped with Tm, Yb, Eu, Er are of most interest as promising multifunctional solids for lasing and non-linear optical applications [1]. So far, no borate of this family is found in the nature, although Italian mineralogists have recently discovered anhydrous rare earth (RE) metaborate with closely spaced chemical composition [2]. For this reason, investigations of crystallogenesis in complex flux systems based on high-temperature RE borates are important from both scientific and technological viewpoints. The present work is focused on flux growth and characterization of  $Y(Ga_xAl_{1-x})_3(BO_3)_4$  (x = 0, 0.05, 0.15, 0.2, 0.4) (YGAB) single crystals. YGAB crystals were obtained by top seeded solution growth technique as wel as spontaneous nucleation under different conditions using a K<sub>2</sub>Mo<sub>3</sub>O<sub>10</sub> based flux. As a result, transparent and homogenous YGAB single crystals with size up to 3 mm have been grown. From ASEM data, it was found that the average Ga distribution coefficients in YGaAB crystals slightly rises from 0.84 to 0.98 with increase of Ga concentration in the initial borates from 5 to 15 at %.

This research was supported, in part, by RFBR grant № 04-05-64709.

[1] Leonyuk N.I., Prog. Crystal Growth and Charact., 1995, 31, 279. [2] Ventura G.D., Parodi G.C., Montana A., Chaussidon M. Eur.Y.Miner., 1993, 5. 53-55

Keywords: boron compounds, crystal growth from solution, crystal characterization

## P.16.04.6

Acta Cryst. (2005). A61, C441-C442

Characterization of Profiled LiNbO3 and SBN Crystals by X-ray Diffraction

Liudmila Ivleva<sup>a</sup>, V. Voronov<sup>a</sup>, M. Samoylovitch<sup>b</sup>, <sup>a</sup>General Physics