

**o.m1.p17** **Structural Features of Flux Grown (Y,RE)Al<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> (RE = Nd, Gd) Solid Solutions.** E.V. Koporulina<sup>1</sup>, N.I. Leonyuk<sup>1</sup>, A.V. Mokhov<sup>2</sup>, <sup>1</sup>Moscow State University, Moscow 119899, Russia; <sup>2</sup>IGEM RAS, Moscow 109017, Russia

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Non-centrosymmetric RE<sub>x</sub>Y<sub>1-x</sub>Al<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> (REYAB) crystals with RE=Nd<sup>3+</sup> and Gd<sup>3+</sup> are of most interest as a promising materials for lasing and non-linear optical applications<sup>1</sup>. These compounds have a good thermal and chemical stability. Due to a possibility of wide isomorphous substitutions, they can be considered as polyfunctional materials with device potential. At the same time, Nd- and Gd-borates also have high temperature monoclinic modifications with the phase transition temperatures of 880-900°C, 1040-1050°C respectively<sup>2</sup>. For this reason, the study of relationships between flux growth conditions, composition, morphology and structure of these crystals are very important. In the present work, the REYAB systems have been studied from this point of view.

Borate crystals were prepared by the TSSG (top seeded solution growth) method as well as spontaneous nucleation using a K<sub>2</sub>Mo<sub>3</sub>O<sub>10</sub> based flux in the temperature ranges of 1120°C - 900°C. The REYAB crystalline substances in the starting solutions were 20 wt%. The composition, homogeneity and external morphology of grown crystals were investigated by the analytical scanning electron microscope JSM-5300 + Link ISIS, analytical transmission electron microscope (ATEM) PEM-125K and the scanning electron microscope (SEM) HITACHI-800.

The SEM photographs show the growth striations developed strongly on the trigonal prism faces of some REYAB crystals obtained by spontaneous nucleation, as opposed to the crystals grown by TSSG method. These striations are parallel to the edges of {10 11} rhombohedra. In the same direction, following to the ASEM measurements, there is a sharp alteration of the layers with the different Gd (Nd) and Y contents. Striations on the trigonal prism faces correspond to boundaries between two kinds of layers. We suppose, the layers enriched in Y<sup>3+</sup> belong to the huntite R32 structure, but the another, monoclinic (C2 or C2/c) modification, has high Gd(Nd) concentration.

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[1] N.I.Leonyuk and L.I.Leonyuk. Growth and characterization of RM<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystals. Prog.Crystal Growth and Chatact (1995), v. 31: 179-278.

[2] E.L.Belokoneva, N.I.Leonyuk et al. Monoclinic modification of rare earth borates. Kristallografiya (1988), v.33: 1287-1288 (in Russian).

**o.m1.p18** **Electronic structure and Pb-O bonding in Complex Lead Perovskites and Lead Monoxide.** J.M. Raulot, P. Cortona and G. Baldinozzi, SPMS, CNRS-Ecole Centrale Paris, Grande Voie des Vignes, 92295 Châtenay-Malabry Cedex, France.

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Complex lead based ferroelectric perovskites are materials of considerable interest both from an industrial and academic point of view. These compounds have found application in several industrial fields as high density capacitors, actuators, pyro-electric detectors and piezo-electric transducers (Lines and Glass 1977).

The prototype structure of perovskite compounds (ABO<sub>3</sub>) is cubic (Pm $\bar{3}$ m) and it consists of oxygen octahedra BO<sub>6</sub> sharing their corners and packed in a three-dimensional array while the A cations occupy the octahedral voids. If two different species of cations, namely B' and B'', are substituted for the B cation, the complex perovskite structure is obtained. The existence of a cationic ordering depends upon the stoichiometry, the charge and the cationic size differences.

Complex perovskite electronic structures are not easily accessible from experiments because of the heavy atoms sitting on the A-site of the structure. Understanding the electronic structure is an obliged step for the understanding of the energetics and electronic structure instabilities responsible for the onset of the ferroelastic and ferroelectric phase transitions. In particular, the covalency character of the bondings has a considerable impact on the softening of the interactions between the different ions in the structure, leading to the eventual appearance of potential minima sitting off of the cubic sites. Depending on the existence or not of this local minima, the phase transition character can be mostly order-disorder or displacive.

We have undertaken self consistent calculations (PWSCF) of the electronic structure, charge distribution and effective charges in lead complex perovskites Pb<sub>2</sub>B'B''O<sub>6</sub> (B'=Mg or Yb and B''= W or Nb) and in lead monoxide in order to better understand the behaviour of Pb-O bonding in these compounds. The analysis of the bonding in these compounds allows us to discuss the common features of lead stereochemistry.