MS81.P38

Acta Cryst. (2011) A**67,** C716

3-D transition metal phosphate zeotypes: controlling dimensionality with chemical substitution

Paul F. Henry,[a] Simon A.J. Kimber,[b] Dimitri N. Argyriou[a] [a] *ESS AB, Lund, Sweden*. [b]*ESRF, Grenoble, France.* E-mail: paul.henry@esss.se

Materials with both magnetic and electric orders such as the magnetoelectric (ME) multiferroics have received significant attention in recent years. [1], [2] The coupling of such behaviours should give rise to technological uses but also lead to rich physics. Often, ferroelectric and magnetic phases have very different ordering temperatures, which suggest that the processes are driven by different microscopic interactions, but for a significant number of materials these coincide and ferroelectricity can be generated by long-range order. Phosphate based materials have been discovered with applications across the whole range of solid state chemistry and physics from battery materials to solid oxide fuel cells and proton conductors. The lithium orthophosphates (LO) $LiMPO_4$ with M = Mn, Fe, Co and Ni are a prototypical iso-structural group of antiferromagnets (AFs) that show ME below their Néel temperatures. [3],[4],[5],[6],[7].

Here we present work on materials of the type $ABPO_4$ with A = Rb and Cs and B = Co, Ni and Cu that show novel frameworks based on structures intermediate between that of zeolite ABW and the natural mineral olivine that have the potential to yield interesting properties. In the Cu system, polymorphic piezo-chromic behaviour is observed at RT driven by coordination changes in the Cu polyhedra. The structure can be locked into one of the polymorphs by doping with Ni and the dimensionality of the structure can be tuned by substitution of the A site cation [8].

[1] S-W. Cheong, M. Mostovoy, *Nature Mater.* **2007**, *6*, 13. [2] D.I. Khomskii, *J. Magn. Magn. Mater.* **2006**, *306*, 1. [3] M. Mercier, Ph.D thesis, Université de Grenoble, **1969**. [4] B.B. van-Aken *et al.*, *Nature (London)* **2007**, *449*, 702. [5] T.B.S. Jensen *et al.*, *PRB* **2009***, 79*, 092412. [6] I. Abrahams, K.S. Easson, *Acta Cryst.* **1985**, *C49*, 925. [7] D. Vaknin *et al., Phys. Rev. Lett.* **2004**, *92*, 207201. [8] P.F. Henry, S.A.J. Kimber, D.N. Argyriou. *Acta Cryst. B* **2010**, *66(4)*, 412.

Keywords: crystallography, magnetism, phosphate

MS81.P39

Acta Cryst. (2011) A**67,** C716

Optical properties of lanthanum – gallium tantalate crystals

N.S. Kozlova,[a] O.A.Buzanov,[b] I.S. Didenko,[a] E.S. Kanaeva,[a] A.P.Kozlova,[a] N.A. Siminel,[a] [a]*National University of Science and Technology "MISIS", Moscow (Russia).* [b]*Company Fomos-Materials, Moscow (Russia).* E-mail: kozlova_nina@mail.ru

Lanthanum – gallium tantalate crystal $La_3Ta_{0.5}Ga_{5.5}O_{14}$ (langatate) is a piezoelectric material with a piezoelectric constant about three times higher than that of quartz and is stable over a wide temperature range. Langatate is LGS-type crystals which have the $Ca_3Ga_2Ge_4O_{14}$ type structure with the P321 space group. This crystal is widely used in design of sensors based on the direct piezoelectric effect. One of the investigation issues of langatate is crystal coloration which depends on the presence of color centers. It is necessary to understand the mechanism and nature of color centers formation in crystals to have influence on formation processes. Growth conditions and heat treatment are factors of great.

In this study, we performed experiments with langatate crystals produced by the company Fomos-Materials. The crystals were grown by the Czochralski method in iridium crucibles in an Ar atmosphere and in a mixture of argon and oxygen (Ar +(2%)O_2) and (Ar +(~0,5%) O_2). Crystals grown in Ar atmosphere are almost colorless, while those grown in (Ar+O_2) atmosphere are of bright orange color.

Presence of point defects in structure and processes of recharge have an influence on color centers formation. It leads to generation of optical active localized states. Formation processes might be activated with additional postgrowth treatment particularly with annealing.

Isothermal annealing in the air was carried out at temperature 500 ^{0}C, 600 ^{0}C, 700 ^{0}C, 800 ^{0}C, 900 ^{0}C, 1000 ^{0}C, each sample was held within 4 hours at only one temperature. The experiment required using the polar cut samples 2 mm thickness. All samples were investigated with methods of optical spectroscopy, optical microscopy, atomic force microscopy, X-ray photoelectron spectroscopy before and after annealing. Optical transmission and diffused reflection spectra were measured with spectrophotometer "Cary 5000 UV-VIS-NIR" in the wavelength range 230-3000 nm and attachment "DRA 2500" for diffused reflection measurements. A strong effect of the annealing temperature on the state of defects in langatate structure and crystal surfaces has been revealed. It depends on the growth atmosphere.

Increased absorption is observed on specific absorption bands at wavelengths 280 nm, 360 nm and 480 nm. Consecutive decrease of transmission coefficient is accompanied by temperature rise.

Measurement by means of optical microscopy demonstrated the fact that annealing leads to significant change of one of the crystal surfaces Optical transmission spectra give integral characteristic measurements of diffused reflection spectra of both surfaces.. Analysis of these spectra shows differences between diffused reflection coefficients of positive and negative surfaces of the samples. It might be connected with unequal structure changing of surfaces.

Results of the surface research by means of X-ray photoelectron spectrometer PHI 5500 ESCA exhibit tendency to decreasing of correlation Ga to La concentrations in samples subjected to annealing at 1000 ^{o}C.

Obtained results are evidence of isothermal annealing having a profound effect on both optical properties and surfaces states in $La_3Ta_{0.5}Ga_{5.5}O_{14}$ crystal. Dependence of surface state on their polarity and the growth atmosphere is observed.

Keywords: annealing, property, optics

MS81.P40

Acta Cryst. (2011) A**67,** C716-C717

Temperature dependent phase transition and topological classification of GdP_5O_{14}

Alisha J. Cramer,[a] Jacqueline M. Cole,[a,b] [a]*Department of Physics, University of New Brunswick, Fredericton New Brunswick, (Canada).* [b]*Cavendish Laboratory, University of Cambidge, Cambridge, (UK).* E-mail: Alisha.Cramer@unb.ca

Porous materials have attracted much interest in their potential to absorb other molecules into the crystal framework for a variety of uses ranging from solar cells to gas recognition and storage [1], [2]. Relationships between temperature and structure geometry often prove to be of great importance in this regard [3].

In a multi-temperature, single-crystal X-ray diffraction study on gadolinium ultraphosphate (GdP_5O_{14}), we have investigated the second-order monoclinic to orthorhombic solid-state phase transition. Temperature measurements ranged from 125K to 480K, and the images were integrated and refined assuming both the monoclinic structural framework, and the orthorhombic framework. The results were then compared and the phase transition was found to be around 350K-400K. This result is consistent with the predictions and results reported from previous ferroelasticity studies [4], [5].