

(XRPD) patterns revealed the new compound to have a vaterite-type and warwickite-type structure, respectively. The modification with vaterite-type structure is known for other rare earth borates, for example, YBO_3 and YbBO_3 , as a stable form. The warwickite-type phase is known for $\text{M}_1^{3+}\text{M}_2^{2+}\text{OBO}_3$ -type compounds. ScBO_3 was believed earlier to have calcite-type structure type only. Non-equilibrium processes during heating-quenching cycles lead to form new metastable phases in ScBO_3 . We carried out detailed studies of ScBO_3 structural transformations by differential scanning calorimetry and *in situ* x-ray powder diffraction techniques. The quenched samples were characterized by IR spectroscopy, as well as XRD. We revealed that non-reversible sequence of amorphous \rightarrow warwickite-type \rightarrow vaterite-type \rightarrow calcite-type transformations took place in the temperature range 1036-1054 K. Total exothermal effect for the amorphous \rightarrow warwickite-type \rightarrow vaterite-type transformations correspond to $\Delta H=142.4$ J/g and that of vaterite-type \rightarrow calcite-type transition is $\Delta H=85$ J/g. The lattice parameters of the ScBO_3 warwickite-type structure are $a=9.4248$ Å, $b=9.4451$ Å and $c=3.3969$ Å, $\beta=90.309$, S.G.= $P2_1/n$ and ones of the vaterite-type structure are $a=3.8952$ Å, $c=7.8772$ Å, S.G. = $P6_3/mmc$, respectively. The details of the crystal structures will be discussed in the presentation.

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Keywords: complex oxides; nanomaterials; X-ray powder diffraction

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Mineral Apatite as a Periodic Model of Surface to Living Cell Growth. Marzena Suder^a, Małgorzata Tyszkiewicz-Czochara^b, Katarzyna Stadnicka^a. ^a*Jagiellonian University, Faculty of Chemistry, Krakow, Poland.* ^b*Jagiellonian University, Faculty of Pharmacy, Krakow, Poland.*

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A mineral apatite, $\text{Ca}_5(\text{PO}_4)_3(\text{F},\text{OH},\text{Cl})$ as a main source of phosphorus in nature, has a great importance in designing materials useful for medical purposes. Moreover, it is worth to say, that the mineral single-crystal apatites can obtain size up to several centimeters [1]. In comparison to above, a calcium deficient carbonate-hydroxylapatite suitable as a mineral part of vertebrates bones, occurs in shape of nano-sized crystals [1,2]. The hydroxylapatite, with a chemical composition similar to biological apatites and its proved biocompatibility, is broadly applied in medicine and stomatology [3]. It is interesting to what extent the different crystallographic orientation of the single-crystal faces has influence on living cell growth. Two types of geological crystals of different origin, with molecular formulas $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_{1.38}(\text{OH})_{0.62}$ (I) and $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_{1.09}(\text{OH})_{0.86}\text{Cl}_{0.05}$ (II), were studied. The material was characterized by various methods – polarizing microscopy, single-crystal X-ray diffraction and energy-dispersive X-ray spectroscopy for the evaluation of surface chemistry. In both cases lattice symmetry was found to be hexagonal with the point group

$P6_3/m$ and following unit cell parameters: $a=9.3839(4)$ Å, $c=6.8867(3)$ Å for (I) and $a=9.4058(4)$ Å, $c=6.8807(3)$ Å for (II). A basis to assume right model of the surface of the following faces: (10-10), (0001) and (10-11) was structural analysis. Subsequently, a chosen cell line of human fibroblasts has been grown on the prepared crystal plates with orientations (10-10), (0001) and (10-11). We hope that the studies will shed light on the understanding of living cell – apatite substrate interactions at atomic level.

[1] Phosphates: Geochemical, geobiological, and materials importance, edited by Kohn M.J, Rakovan J., Hughes J.M., Reviews in *Mineralogy and Geochemistry*, vol. 48, Mineral. Soc. Am. **2000**. [2] Glimcher M.J. Bone: Nature of the Calcium Phosphate Crystals and Cellular, Structural, and Physical Chemical Mechanisms in Their Formation, Reviews in *Mineralogy & Geochemistry*, **2006**, 64, 223. [3] Biomaterials Science An Introduction to Materials in Medicine, edited by Ratner B.D., Hoffman A.S., Schoen F.J., Lemons J.E., Elsevier Academic Press **2004**, 2nd edition.

Keywords: biomaterials; apatites; single-crystal X-ray diffraction

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Kinetics of the Dehydroxylation and Mullitization Processes of Nanotubular Halloysite Mineral.

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A mineral clay deposit from the locality “Guelma”, was investigated. The exploitation of the results of chemical, X-rays, IR and differential thermal analyses shows that the raw material is essentially formed with halloysite. Examined with S.E.M., the clay particles have a nanotubular form with 100 to 300nm in length and 20 to 50 nm in external diameter. The activation energy of dehydroxylation was determined as 160 kJ.mol⁻¹, while the value for mullitisation is 844 kJ.mol⁻¹.

Keywords: halloysite; natural nanotube; kinetics of dehydroxylation

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Defects in Fluorite Structure Caused by Natural Irradiation. Vojtěch Vlček^e, Roman Skála^a, Jakub Čížek^d, Jan Drahoukoupil^b, Jan Valenta^c, Jana Ederová^f, Viktor Goliáš^e. ^a*Academy of Sciences of the Czech Republic, v.v.i. Institute of Geology, Prague, Czech Republic.* ^b*Academy of Science of The Czech Republic, v.v.i., Institute of Physics, Prague, Czech Republic.* ^c*Charles University in Prague, Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic.* ^d*Charles University in Prague, Department*

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Artificially irradiated CaF₂ (recently studied) may not be a proper analogue to fluorite irradiated for a long-time in order of millions of years under natural conditions. Naturally irradiated fluorite samples have been analyzed by means of X-ray powder diffraction analysis (XRD), Differential Scanning Calorimetry (DSC), Positron annihilation spectroscopy (PAS) and Photoluminescence Spectroscopy. Results have shown that the unit cell volume of all irradiated samples is slightly increased (0.26% at maximum). Evaluation of the diffractogram of the highly irradiated samples using Williamson-Hall method showed micro-strain about 0.13% but no change in crystallinity was observed at the same time. The micro-strain values were in different samples almost invariant and may therefore represent the micro-strain saturation value. Based on results from XRD and PAS, presence of dislocation loops and vacancy clusters causing strain in the structure is assumed. The high density of defects is showed by PAS where saturated positron trapping is observed. Laboratory sample annealing has shown that the structure reconstruction begins between 300°C and 400°C when strain value decreases rapidly but further increase of temperature does not affect micro strain and its value remains higher than in the non-irradiated samples. DSC analysis showed exothermic peak at 273°C and represents enthalpy change about 200 J.g⁻¹ that exceeds calculated change due to unit-cell volume increase. All irradiated samples are purple; this could be ascribed to various types of colour centres. During heating the colour change is observed (annealed samples are colourless) as well as the change of photoluminescence spectra.

Keywords: fluorite; defect; irradiation

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Reversible Phase Transition in Precious Metal-doped LaMnO₃ Perovskites. Dominic Stuermer^a, Lars Giebeler^a, Hartmut Fuess^a. ^aDepartment of Material Science, University of Technology Darmstadt.

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In Pd-containing LaMnO₃ perovskites, a reversible phase transition appears during *in situ* cycling with hydrogen monitored by synchrotron X-ray powder diffraction [1]. This phase transition is strongly dependent on the noble metal addition. Otherwise, it seems to be independent of the gas atmosphere which is shown for H₂, O₂ and air. Even very small Pd-contents promote the change from the trigonal space group *R*-3c to the orthorhombic space group *Pnma* at about 650 °C. The phase transition is also found

for other precious metals like Pt, Rh or Ru but not for the undoped LaMnO₃.

Lattice constants develop independency on the temperature until the phase transition occurs. Above this temperature, a significant increase of the lattice constants of the trigonal phase is observed.

Recent studies aim on the location of the precious metal atoms in the perovskite lattice. To locate the atoms position precisely, additionally to X-ray powder diffraction, transmission electron microscopy with energy-dispersive X-ray spectroscopy and Raman spectroscopy are applied.

[1] D. Stuermer, L. Giebeler, C. Baecht, H. Fuess; *Europcat VIII Turku 2007*; P14-55

Keywords: lanthanide oxides; solid-state phase-transition; noble metals

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Gallery of Back-Reflection Laue Images of Some Optical and Magnetic Crystals. Jiří Hybler. *Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18221 Praha 8, Czech Republic.*

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The Laue method is historically the oldest method of X-ray diffraction. It has been soon eclipsed by more sophisticated moving-crystal methods, and later by the development of the diffractometry.

The unfiltered (polychromatic) X-ray beam hits the stationary crystal and diffracted beams are recorded on the (usually planar) film or image plate. The Bragg condition is obeyed for an a priori unknown wavelength corresponding to the given *d* and fixed *θ* of the respective lattice plane. The method provides collapsed and distorted image of the reciprocal lattice [1]. Diffraction spots are arranged on cone sections – ellipses and hyperbolae for the front- and back-reflection arrangements, respectively. These cone sections correspond to the zones in direct space and planes in the reciprocal lattice.

For various optical and magnetic studies, oriented single crystals in form of prisms or plates are required. The back-reflection Laue method is an appropriate method to set bulk crystals (fixed in some kind of a special holder allowing rotations and/or tilting in a certain extent) into the defined position with respect of crystallographical axes. The holder together with the oriented crystal can be then mounted onto the saw and oriented specimens can be prepared by cutting. The back-reflection arrangement allows checking crystals of theoretically unlimited size. However, the diffraction pattern is relevant to the irradiated area only.

The distribution of diffraction spots and of hyperbolae reflects the Laue symmetry around the symmetry elements parallel to the primary beam. This arrangement is usually characteristic for given crystalline substance, orientation, and experimental conditions. The poster presents a gallery of characteristic back-reflection Laue pattern of several crystals important for optical and magnetic studies, e.g. of PbWO₄ (PWO, tetragonal, scheelite structure), YAlO₃