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Artificially irradiated CaF_2 (recently studied) may not be a proper analogue to fluorite irradiated for a long-time in order of milions 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. Lanoratory 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

FA2-MS02-P09

Reversible Phase Transition in Precious Metal-doped $LaMnO_3$ Perovskites.

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In Pd-containing $LaMnO_3$ 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 H**2, O_2** and air. Even very small Pd-contents promote the change from the trigonal space group *R*-3c to the orthorhombic space group *P*nma at about 650 °C. The phase transition is also found for other precious metals like Pt, Rh or Ru but not for the undoped $LaMnO_3$.
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 atome 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. Baehtz, 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.

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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 $PbWO_4$ (PWO, tetragonal, scheelite structure), $YAlO_3$

(YAP, orthorhombically distorted perovskite structure), yttrium aluminium garnet (YAG, cubic), Lu_2SiO_5 (LSO, monoclinic), and of magnetite (spinel structure).

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Keywords: laue diffraction; optical materials; magnetic materials

FA2-MS02-P11

Control of Morphology, Size and Porosity of The Zinc Oxide by Chemical Additives.

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In biological and synthetic systems, control of crystal morphology, porosity and size are very important. Many works focused different types of minerals, including $CaCO_3$, TiO_2, ZnS, ZnO, CdO, etc. [1] Zinc oxide (ZnO) is a unique material that exhibits semiconducting, piezoelectric, and pyroelectric multiple properties. Numerous chemical strategies have been reported to synthesize including controlled precipitation, hydrothermal and solvothermal methods, sol–gel, thermal decomposition of precursors, laser ablation, spray pyrolysis, oxidation of zinc metal, and microemulsion [2-6]. But many of these methods usually require high temperature. Therefore, it is important to develop processes for continuous production of uniform particle size distribution based on precise specifications for given use in low temperature. In this work, ZnO crystals have been prepared by mixing aqueous solutions of zinc nitrate and Hexamethylenetetramine (HMT) in the presence of latex particles and green polymer. Latex is an aqueous microemulsion based on styrene-acrylic copolymer. Polymer is environmentally friendly polysaccharide-based polycarboxylate, carboxymethyl inulin (CMI). Zinc oxide (ZnO) were synthesized by homogeneous precipitation method and were characterized by SEM, X-ray diffraction analysis, BET and zeta sizer. The effects of the latex particles and green polymer on the crystal growth, morphology and crystalline structure of the resulting zinc oxide were studied by SEM, X-ray diffraction analysis, BET and zeta sizer. The additives affect the dimension, morphology and particle size distribution of the crystals. The reduction in size is greater in the direction of the c-axis. The SEM micrograph shows the formation of well-crystallized, agglomerated small particles of ZnO. The mean size of the subunit determined by XRD is smaller than that of the surface of the grain observed in SEM. The porous ZnO were mainly manufactured by removal of the additives via heat treatment. The additive concentration, sintering time and sintering temperature were varied to investigate their influence on the quality of the porous matrix.

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Keywords: zinc compounds; crystallization; biopolymers

FA2-MS02-P12

Synthetic Dimetaborates *REE*Al$_{1.67+0.67x}$(B$_4$O$_{10}$)O$_x$ (x ≤ 1) (*REE* = La, Ce, Nd, Pm, Sm, Eu): Crystal-Chemical Study and Comparison with Natural Counterpart Peprossiite-(Ce).

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In the present work we relate a crystal chemical study of a series of synthetic dimetaborates with composition *REE*Al$_{1.67+0.67x}$(B$_4$O$_{10}$)O$_x$ (x ≤ 1) [1] (*REE* = La, Ce, Nd, Pm, Sm, Eu) performed by single-crystal X ray diffraction. The samples were obtained by slow cooling from $K_2Mo_3O_{10}$ based fluxed melts in the form of transparent hexagonal sheet-like crystals. Structure refinements showed all the phases to be isostructural within hexagonal space group P-*62m* with mineral peprossiite-(Ce) (a = 4.612(1) Å; c = 9.374(3) Å and V = 172.6 Å^3) [2], a late pegmatitic - hydrothermal phase from holocrystalline ejecta of the Vico volcanic complex (Italy). The *REE* cations present a trigonal prismatic coordination; Al cations are surrounded by five oxygen atoms, resembling a square pyramidal coordination, BO_4 groups display tetrahedral arrangement. The three-dimensional framework can be described as a packing of *REE*O$_6$, BO_4 and AlO_5 polyhedral layers perpendicularly to the crystallographic c axis, held together by strong *REE*…O and Al…O interactions.

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Keywords: dimetaborates; rare earth elements (*REE*); peprossiite-(Ce)

FA2-MS02-P13

Influence of F$^-$/OH$^-$ Exchange on the Morphology of Apatite-Gelatine-Composites.

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Biomimetic apatite–gelatine nanocomposites are grown in a double diffusion setup, where calcium chloride and disodium hydrogen phosphate / sodium fluoride stock solutions diffuse through a gelatine gel from opposite ends under controlled temperature conditions. Composite aggregates are found in periodic growth zones within the gel (Liesegang Bands) and exhibit a hierarchical resemblance to apatite-collagen system found in bone and teeth [1].