

of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic. ^aCharles University in Prague, Institute of Geochemistry, Mineralogy and Mineral Resources, Prague, Czech Republic, ^fInstitute of Chemical Technology, Laboratory of Thermal Analysis, Prague, Czech Republic.

E-mail: vojtech.vlcek@gmail.com

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

FA2-MS02-P09

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.

E-mail: dominic@st.tu.darmstadt.de

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

FA2-MS02-P10

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.*

E-mail: hybler@fzu.cz

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