positions. A well studied phase transition from A2/a – $P2_1/a$ occurs near 500 K. In nature titanite often incorporates various impurities like the radiogenic elements U and Th. Through the resulting structural damage induced by α- and β-decay the titanite becomes metamict. This means over geological time scales recoil processes due to alpha radiation change the originally periodically structured material into a quasi-amorphous state with persisting short-range order but destroyed long-range order. We present IR and Raman spectra as well as X-ray diffraction data of metamict and heat treated titanite from the Cardiff mine in Canada. The Raman and IR modes are strongly broadened in the metamict material and became sharper on annealing. The OH-stretching mode at 3486 cm^{-1} indicates strong changes in the local environment of OH^- in metamict titanite. Between 620 and 750 cm^{-1} Raman excitations appear in the metamict material, which in IR spectra result from Ti-O stretching excitations of the TiO_6 octahedra. This indicates the breakdown of the Raman selection rules and points to the breaking of the octahedral symmetry of TiO_6 polyhedra.

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Keywords: titanite, metamict, x-ray diffraction

FA2-MS16-P19

Crystal chemistry of synthetic semiconductors $Pb_5Sb_4S_{11-m}X_m$ (X=Te,Se). Klaus Bente[a], Gerald Wagner[a], Ronny Kaden[a], Sven Gerhardt[a], Sandra Lobe[a]. [a]*Institut für Mineralogie, Kristallographie und Materialwissenschaft, University of Leipzig, Germany*
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Inspired by the natural semiconductor boulangerite, $Pb_5Sb_4S_{11}$, the sulfosalts $Pb_5Sb_4S_{11-m}Se_m$ and $Pb_5Sb_4S_{11-m}Te_m$ of varying compositions ($0.0< m < 11$, step width of m = 1) were synthesized by solid state reaction.
The chemical composition was determined by powder X-ray diffraction and electron microprobe analysis. If the Se and/or Te content is increased the Pb(Pb+Sb) ratio decreases. X-ray powder diffraction was used to determine lattice parameters related to the composition.
The synthesized powders were used as starting material for single crystal growth via chemical vapour transport. Iodine was used as transporting agent.
To determine the composition of the as-grown single crystals both REM-EDX and TEM-EDX were applied. The electrical conductivity of these needle-shaped single crystals improves with increasing selenium and/or tellurium content.

Keywords: semiconductor, lattice parameters, boulangerite

FA2-MS16-P20

Comparative study of the stability of various crystallographic phases with composition and stress in the multiferroic $BiFeO_3$-x$PbTiO_3$ system. Shuvrajyoti Bhattacharjee[a], Dhananjai Pandey[a]. [a]*School of Materials Science and Technology, Banaras Hindu University, Varanasi, 221005.*
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$BiFeO_3$ (BF) is an attractive multiferroic material, exhibiting antiferromagnetic [G-type, having an incommensurate cycloidal spin structure] transition at T_N ~ 643 K and a ferroelectric transition at T_C ~ 1103 K. $BiFeO_3$ forms a continuous solid solution with $PbTiO_3$ and shows a morphotropic phase boundary (MPB) region. There is considerable controversy in literature about the location, width and constituting crystallographic phases of the MPB in the (1-x)$BiFeO_3$-x$PbTiO_3$ (BF-xPT) system[1,2]. Also in this system applied external stress can induce a tetragonal phase in the Bi rich side of MPB and this effect can effectively alter the width of the MPB[3]. We have studied the stability of various crystallographic phases of (1-x)$BiFeO_3$-x$PbTiO_3$ (BF-xPT) as a function of composition and applied stress and have established accurately the room temperature phase diagram for this solid solution[4,5,6]. It is shown that the structure of BF-xPT is tetragonal for $x>0.31$ in the P4mm space group and monoclinic for $0.10\leq x\leq 0.27$ in Cc space group, whereas the two phases coexist in the MPB region $0.27<x<0.31$.[4,5]. The composition width, $\Delta x \sim 0.03$, for the MPB observed by us is the narrowest reported so far in the literature for this system. We have shown that the very high c/a ratio in the tetragonal phase of this system is linked with the covalency effects for bonding between both A and B site cations with oxygen, by comparing the observed bond lengths between oxygen and other cations, obtained from Rietveld analysis of the room temperature powder x-ray diffraction data with expected ionic bond lengths. We have studied the nature of stress induced phase transition for compositions on the $BiFeO_3$ rich side and shows that the width of the MPB region is extended as a result of external stress. It has been found that this effect is most prominent for compositions close to the MPB, reduces with increasing $BiFeO_3$ content and for x=0.9 the effect is practically absent. But there is no similar effect on the tetragonal side of the MPB. A high temperature x-ray diffraction study carried out on x=0.27 composition (which has a monoclinic structure with Cc space group symmetry) with stress induced tetragonal phase shows that the stress induced tetragonal phase and the parent monoclinic phase both transform to paraelectric cubic phase simultaneously.

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Keywords: Multiferroic, Perovskites, Rietveld refinement.

FA2-MS16-P21

Environmental Aspects of Mineral Synthesis Through Interaction of Smoke Gases from Biomass Burning and Low Grade MnO_2 Ores. A.F. Bishay, R.S. Moharb. *Nuclear Materials Authority, Cairo, Egypt.*
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The biomass burning results a mixture of gases and particulate matter [1] causing hazardous air pollution as the so called black clouds left behind rice straw. In this study, low grade lumps and dust of manganese oxides capture effectively the evolved gases from the rice straw burning. The rice straw