positions. A well studied phase transition from A2/a \rightarrow P21/a occurs near 500 K. In nature titaneite often incorporates various impurities like the radiogenic elements U and Th. Through the resulting structural damage induced by α- and β-decay the titaneite 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 titaneite 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 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.

We have established accurately the room temperature phase diagram for this solid solution\(^4,5\). It is shown that the structure of BiFeO\(_3\)-xPbTiO\(_3\) (Bi-xPT) as a function of composition and applied stress and have established accurately the room temperature phase diagram for this solid solution\(^1\)\(^–\)\(^5\). 

**Keywords:** titaneite, metamict, x-ray diffraction

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**FA2-MS16-P19**

Crystal chemistry of synthetic semiconductors Pb\(_5\)Sb\(_4\)S\(_{11}\)-xTe\(_x\) (x=Te,Se), Klaus Bente\(^1\), Gerald Wagner\(^2\), Ronny Kaden\(^2\), Sven Gerhardt\(^2\), Sandra Lobe\(^3\).

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Influenced by the natural semiconductor boulangerite, Pb\(_5\)Sb\(_4\)S\(_{11}\), the sulfosalts Pb\(_5\)Sb\(_4\)S\(_{11}\)-xTe\(_x\) and Pb\(_5\)Sb\(_4\)S\(_{11}\)-xTe\(_x\) of varying compositions (0.0\(<\ x\ <\ 1\), 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

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**FA2-MS16-P20**

Comparative study of the stability of various crystallographic phases with composition and stress in the multiferroic BiFeO\(_3\)-xPbTiO\(_3\) system, Shuvrajyoti Bhattacharjee\(^4\), Dhananjai Pandey\(^4\). "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 \(T_N\sim 643\) K and a ferroelectric transition at \(T_C\sim 1103\) 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\(_3\)-xPbTiO\(_3\) (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\(^3\).\(^4\). We have studied the stability of various crystallographic phases of (1-x)BiFeO\(_3\)-xPbTiO\(_3\) (BF-xPT) as a function of composition and applied stress and have established accurately the room temperature phase diagram for this solid solution\(^5\),\(^6\).


**Keywords:** Multiferroic, Perovskites, Rietveld refinement.

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**FA2-MS16-P21**


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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...
residual ash is enriched in silica and applied as a good adsorbent material for heavy metals [2]. The capture of carbon dioxide and other smoke gases from the biomass burning can be vitally achieved through hot manganese oxide at 200-250°C. The gases change the biomass burning can be vitally achieved through hot manganese oxide at 200-250°C. The gases change the mineralogical composition of the applied manganese oxides as investigated by using XRD, IR and SEM-EDX analysis. The environmental impact of the process can be deduced from the significant change in the mineralogy of the manganese ore from mainly oxide forms to carbonate and halide rich phases. The ore impurities (e.g. Na, Mg, Ca, Al and F ) contribute largely in the obtained mineral phases.


Keywords: CO₂-sequestration, biomass burning, manganese mineralogy.

FA2-MS16-P22
Saccharide Yield From Interacted Biomass With Oxide Minerals For Separation and Fractional Crystallization In Acidic Route Of Mineral Processing. A.F. Bishay. Nuclear Materials Authority, Cairo, Egypt. E-mail: abram_bishay2002@yahoo.com

Voluminous bio-wastes are resulted every year from agriculture where extensive literature review the article of their acidic dissolution [1]. The presence of organic matter represent a triggering factor that controls mineral dissolution in the acid sulfate soil [2]. For implications, rice straw is very promising material in the sulfate medium of mineral processing. The dissociated biomass promotes dissolution, separation and crystallization of oxide minerals avoiding the extra cost. Under controlled boundary conditions and at room temperature, rice straw in dilute sulfate medium using sulfuric acid and manganese oxide yield saccharides and manganese sulfate crystals. Moreover, under drastic acidic conditions and biomass subjection into ilmenite sulfate process, reduced sulfate crystals. Moreover, under drastic acidic conditions and biomass subjection into ilmenite sulfate process, reduced saccharide is obtained with the facility of continuous crystallization of iron sulfate off. The end-product is a cheap and chemically controlled nano-TiO₂ which find many photocatalysis applications.


Keywords: Biomass, mineral processing, saccharides.

FA2-MS16-P23
AI/Si-ordering phenomena in sanidine megacrysts from the Eifel. Kathrin Demtröder, Sara Dehn, Michael Gopon, Jürgen Schreuer. Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum, Germany. E-mail: schreuer@rub.de

Sandine megacrysts from Volkesfeld (Rieden eruptive centre, East Eifel volcanic field, Germany) are well known for their unusual optical properties [1]. Starting from 1025 K their optic axial angle 2V' changes rapidly at higher temperatures. This macroscopic effect has been interpreted as being associated with a corresponding increase of the Al/Si-disorder on the atomic level. The sandines from Volkesfeld are further characterised by very low concentrations of dislocations indicating hydrothermal growth conditions [3]. However, the reason for the drastic and irreversible change of the optical properties is still under debate.

To clarify the role of water and chemical composition for the observed optical anomalies, the Al/Si-ordering has been investigated in sanidine megacrysts from four different eruptive centres of the Eifel and from Madagascar (served as reference) by means of single crystal X-ray diffraction, optical techniques and NMR-spectroscopic studies. The chemical composition Na₂K₁₋ₓAlSi₃O₈ as obtained by electron microprobe analysis, is characterised by x ≈ 0.15 and x > 0.27 for megacrysts from the East Eifel and West Eifel volcanic field, respectively, with up to 2 at-% celiax and less than 0.02 at-% anorthite. The H₂O content varies about between 250 ppm and 400 ppm. All investigated Eifel sandines show irreversible optical anomalies at temperatures above 1073 K. Their optical axis angles 2V' change drastically from about 30° in a plane perpendicular to (010) to about 35° within (010). According to [2] this corresponds to a decrease in the Al/Si order from 2x ≈ 0.70 to 0.58. However, tetrahedral bond distances derived from single crystal structure analyses indicates 2x ≈ 0.58 [4] for fresh samples and only small changes after annealing. The latter findings are supported by ₂⁹Si and ₂⁷Al NMR-experiments. Our contradictory experimental observations are probably caused by the water dissolved in the crystal structure of these nominally anhydrous minerals.


Keywords: AI/Si-ordering, sanidine megacrysts, optical anomalies.

FA2-MS16-P24
Core-Shell Ni₅₋ₓTiOPO₄₋ₓ/C Composites as Anode Materials in Li Ion Batteries. Rachid Esselhi², Brahim ElBalib², Zehn Zhou², Hartmut Fues³, "SUBATECH, Unité Mixte de Recherche 6457, École des mines de Nantes, CNRS/IN2P3, Université de Nantes, BP 20722, 44307 Nantes cedex 3 France, ²Laboratory of Mineral Solid and Analytical Chemistry “LMSAC”, Department of Chemistry, Faculty of Sciences, University Mohamed I, PO Box 624, 60000 Oujda, Morocco, ³Institute of New Energy Material Chemistry, Key Laboratory of Advanced Micro/Nanomaterials and Batteries/Cells (Ministry of Education), Nankai University, Tianjin

[2] this corresponds to a decrease in the Al/Si order from 2x ≈ 0.58 

Keywords: AI/Si-ordering, sanidine megacrysts, optical anomalies.