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Sanjuanite, $Al_2(PO_4)(SO_4)OH{\cdot}9H_2O$, is a fibrous mineral found in Carboniferous slates at the Pocito Department, San Juan province, Argentina. This phase was first described in [1] and is chemically related to other hydrated aluminium phosphate-sulphate minerals like kribergite $Al_5(PO_4)_3(SO_4)(OH)_4{\cdot}2H_2O$ [2] and hotsonite $Al_{11}(PO_4)_2(SO_4)_3(OH)_{21}{\cdot}16H_2O$ [3]. Unfortunately, the structural relationship among these minerals is difficult to establish, since no specimens suitable for single-crystal experiments are available, and no isostructural materials are known. To increase the knowledge on these compounds, the crystal structure of sanjuanite was solved and refined from intensity data collected on a conventional powder diffractometer (Bragg-Brentano geometry, scintillation detector, secondary graphite monochromator, $CuK\alpha_{1,2}$ radiation). The first necessary step was the indexing of the powder pattern. Unlike the triclinic unit cell previously proposed in [4], the new monoclinic cell a=14.3719(3), b=17.2381(4), c=6.1110(2) Å, β=106.617(21)º, $V\cong$ 1452 Å^3 indexes all reflections and hence was used for extracting the integrated intensities down to a d-spacing of 1.30 Å. This data set was further processed with S-FFT based direct methods [5]. With the exception of one O atom, all non-H atoms clearly showed up in the Fourier synthesis computed with the refined phases from the best direct methods solution. Once the crystal structure model was completed, it was optimized by restrained Rietveld refinements to an effective χ^2 value of 2.08 [6]. During the refinement the slight preferred orientation along [-2 0 3] detected in the flat sample was treated with the March-Dollase correction. The structure of sanjuanite (space group $P2_1/a$, Z= 4) is composed of infinite alumino-phosphate chains running parallel to c. Isolated $(SO_4)^{2-}$ groups and H_2O molecules connect the groups of chains. Hydrogen bonding plays a key role in the stabilization of the structure.

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Keywords: sanjuanite, ab-initio solution, powder diffraction

FA2-MS16-P14

High resolution phase analyses and early crystallization processes of cement. Moritz-C. Schlegel[a], Urs Mueller[a], Ulrich Panne[a], Franziska Emmerling[a]. [a]*BAM Federal Institute of Materials Research and Testing, Berlin, Germany Materials Science, Technical University Darmstadt, Germany.*
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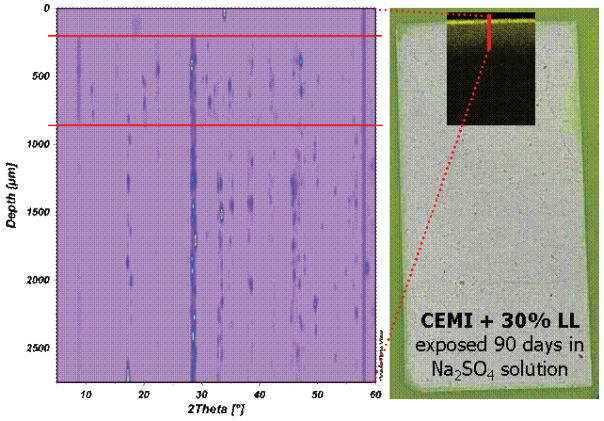
Cementitious building materials are a substantial part of our built environment. Due to the nature of the cementitious binder those materials can be described as multi component nano composite materials. Furthermore, for studying degradation mechanisms spatial chemical or phase analytical data are needed, which can be linked to the microstructure of the cementitious paste. The objectives of this work are the observation of the early crystallization of cement during the hydration and the analysis of the phase assemblage of chemical attacked mortar and concrete including synchrotron methods. Both objectives were examined by diffraction with synchrotron radiation in transmission geometry (λ=1.0656 Å, μ-spot beamline, BESSY II, HZB, Berlin). The latter one is performed using an ultrasonic trap. That was provided the contact free analysis of a sample and ensures a constant water cement ratio. This is a tremendous improvement since former studies using capillaries coupled with water injection system could not guarantee a homogeneous dispersion of water within the cement suspension. The integration time for a single diffraction pattern was about 30 sec and allowed a detailed view into the dynamics of the crystallization processes at early stages. The spatial phase analysis was performed on cement paste and mortar specimens, which were exposed to sulphate and chloride solutions. The reaction fronts of sulphur and chloride were localised by elemental mapping with a micro X-ray fluorescence analysis. Synchrotron X-ray diffraction was used in-situ for the identification of the phase composition (Fig. 1). The primary focussing optics established a spatial resolution of 10 μm for thick section samples with a thickness of ca. 200 μm. That means phase analysis can be performed in-situ with a high local resolution and within the intact micro structure of the sample. First results show patterns with a good peak to background ratio. The measurement of sulphate content exposed cement paste samples reveal a phase composition, determined by synchrotron XRD which corresponds well to the chemical profile measured by micro XRF.



Keywords: cement, time-resolved, space-resolved

FA2-MS16-P15

Elastic anomalies and electromechanical properties of tourmalines. Chandra Shekhar Pandey, Jürgen Schreuer. *Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum, Germany.*
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Tourmalines exhibit a broad variability in chemical composition and are a promising piezoelectric material for acoustic-electronic devices operating at high-temperatures. In contrast to α-quartz, $LiNbO_3$ and materials of the langasite family, the application of tourmaline at temperatures up to its melting point is not limited by phase transitions, electrical conductivity or strong ultrasound dissipation effects.
Here we report the full set of elastic and piezoelectric constants of five natural single crystal tourmalines of gem quality between room temperature and 903 K as determined