

assume a minimum of melting point in the compositional range around  $\text{Sm}_{0.6}\text{Ce}_{0.4}\text{PO}_4$ . First results particularly related to crystal structure analysis of the investigated ceramics will be presented.

[1] G.R. Lumpkin, *Elements* **2006**, 2, 365-372. [2] A. Meldrum, L.A. Boatner, R.C. Ewing, *Physical Review B* **1997**, 56, 13805-13814. [3] E.H. Oelker, F. Poitrasson, *Chemical Geology* **2002**, 191, 73-87. [4] H. Meysamy, K. Riwozki, A. Kornowski, S. Naused, M. Haase, *Advanced Materials* **1999**, 11, 840-844.

**Keywords:** monazite ceramics, structure analysis, nuclear waste

## MS39.P21

*Acta Cryst.* (2011) **A67**, C496

### Raman spectra of Synthetic Orthophosphates used for Nuclear Waste Management

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One of the central tasks in nuclear waste management is the safe conditioning of actinides like e.g. U, Th or Pu resulting from the re-processing of nuclear fuel. Besides borosilicate glasses promising candidates to accomplish that task safely are ceramic orthophosphates that own the crystal structure and properties of the mineral monazite. Monazite is monoclinic (SG  $P2_1/n$ ) and exhibits an extraordinary chemical durability and radiation resistance [1,2,3]. For the development of new conditioning matrices orthophosphates with compositions  $\text{LnPO}_4$  (Ln = La, Ce, Nd, Sm, Eu) were synthesized as first simulation phases without incorporated actinides. These phases were partly radiated by the bombardment with heavy Kr-ions in order to simulate radiation damage caused by  $\alpha$ -emitters ( $\alpha$ -recoil effect).

The quality of all phases (radiated and non-radiated) was first characterized by powder x-ray diffraction. The short range order and medium range order was investigated by raman spectroscopy. Using this technique structural changes due to radiation damage can be detected quite easily [4,5,6]. Resulting raman spectra show a high resolution and allow the discrimination of up to 30 different raman frequencies.

As a first result significant correlations between chemical composition, crystal structure, radiation damage and thermodynamic properties of the investigated ceramics can be detected and will be demonstrated in detail.

The findings of our investigation will be the basis for the further development and evaluation of *real* monazite-type conditioning ceramics containing larger amounts of the actinides U, Th, Pu, Am, Cm and Np.

[1] A. Boatner, B.C. Sales, In: W. Lutze, R.C. Ewing (Eds.): *Radioactive waste forms for the future*, Amsterdam, North-Holland **1988**. [2] G.R. Lumpkin, *Elements* **2006**, 2, 365. [3] W.J. Weber, A. Navrotsky, S. Stefanovsky, E.R. Vance, E. Vernaz, *MRS Bulletin* **2009**, 34, 46. [4] G.M. Begun, G.W. Beall, L.A. Boatner, W.J. Gregor, *J. of Raman Spectroscopy* **1981**, 11, 273. [5] E.N. Silva, A.P. Ayala, I. Guedes, C.W.A. Paschoal, R.L. Moreira, C.-K. Loong, L.A. Boatner, *Optical Materials* **2006**, 29, 224. [6] L. Nasdala, R. Grötzschel, S. Probst, B. Bleisteiner, *Canadian Mineralogist* **2010**, 48, 351.

**Keywords:** raman, monazite ceramics, nuclear waste

## MS39.P22

*Acta Cryst.* (2011) **A67**, C496

### XRD analysis of the corrosion products of research reactor fuel elements

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Corrosion experiments of unirradiated  $\text{UAl}_x\text{-Al}$  and  $\text{U}_3\text{Si}_2\text{-Al}$  research reactor fuel elements were carried out under repository relevant conditions in order to identify and quantify the secondary phases formed by reactions with formation waters being expected in final repositories due to an accidental influx from the enclosing salt formations. This analysis is important for safety assessment issues as such phases quantitatively may act as a barrier against the migration of the released radioactive inventory. In detail the anaerobic experiments were carried out in glass autoclaves at 90°C in repository relevant solutions of defined composition [1]. After termination of the corrosion period WAXS measurements and Rietveld analysis were the major methods being applied for the identification and quantification of the crystalline and amorphous corrosion products which have been subdivided into different grain size fractions previously.

The corrosion products, i. e. the secondary phases of the research reactor fuel elements were identified via "Search/Match" database retrieving. The identified phases were LDH structures, lesukite (aluminium chlorohydrate), elemental iron, residues of uncorroded nuclear fuel, and different iron containing phases like akaganeite, goethite, and lepidocrocite. The quantitative analysis showed that LDH compounds and lesukite are the major crystalline phases which are observed. Rietveld analysis also revealed the content of amorphous phases. To account for an accurate determination of the phase quantities, i. e. for the application of the Brindley [2] correction the average particle diameter has previously determined by REM and image analysis.

For safety assessments the potential for retention of radionuclides has to be focused on the sorption capacities of the major phases as these may additionally applied as a backfilled barrier in order to prevent the migration of radionuclides out of the final repository in deep geological formations.

[1] H. Curtius, G. Kaiser, Z. Paparigas, B. Hansen, A. Neumann, M. Klinkenberg, E. Müller, H. Brücher, D. Bosbach *Reports of the Research Center Jülich, Jülich-4333* **2010**. [2] G.W. Brindley *Phyl. Mag.*, **1945**, 36, 347-369.

**Keywords:** radioactivity, corrosion, waxes, rem

## MS39.P23

*Acta Cryst.* (2011) **A67**, C496-C497

### Stability and Conductivity of Ce-doped Pyrochlores for SOFCs applications

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Solid Oxide Fuel Cells (SOFCs) are highly efficient and environmentally friendly energy conversion devices with a large variety of potential applications. A SOFC has 3 main components: the cathode, which has to have high electronic/ionic conductivity, to be chemically compatible with other cell components, stable in oxidizing atmospheres and a thermal expansion coefficient similar to other components; the electrolyte that should be ionically conductive, electronically insulating, chemically stable at high temperatures and in reducing and oxidizing environments, free of porosity and with thermal expansion that matches electrodes and finally, the anode which should be electrically conductive, stable in reducing atmosphere and should have high electrocatalytic activity, similar thermal expansion