

(YAP, orthorhombically distorted perovskite structure), yttrium aluminium garnet (YAG, cubic), Lu_2SiO_5 (LSO, monoclinic), and of magnetite (spinel structure).

[1] Amoros, J.L., Buerger, M.J., Amoros, M.C.: The Laue method, Academic Press New York-San Francisco-London, 1975.

Keywords: laue diffraction; optical materials; magnetic materials

FA2-MS02-P11

Control of Morphology, Size and Porosity of The Zinc Oxide by Chemical Additives. Bora Akin^a, Mualla Oner^a. ^a*Yildiz Technical University, Chemical Engineering Department, Istanbul-Turkey.*

E-mail: boakin@yildiz.edu.tr

In biological and synthetic systems, control of crystal morphology, porosity and size are very important. Many works focused different types of minerals, including CaCO_3 , TiO_2 , ZnS , ZnO , CdO , etc. [1] Zinc oxide (ZnO) is a unique material that exhibits semiconducting, piezoelectric, and pyroelectric multiple properties. Numerous chemical strategies have been reported to synthesize including controlled precipitation, hydrothermal and solvothermal methods, sol-gel, thermal decomposition of precursors, laser ablation, spray pyrolysis, oxidation of zinc metal, and microemulsion [2-6]. But many of these methods usually require high temperature. Therefore, it is important to develop processes for continuous production of uniform particle size distribution based on precise specifications for given use in low temperature. In this work, ZnO crystals have been prepared by mixing aqueous solutions of zinc nitrate and Hexamethylenetetramine (HMT) in the presence of latex particles and green polymer. Latex is an aqueous microemulsion based on styrene-acrylic copolymer. Polymer is environmentally friendly polysaccharide-based polycarboxylate, carboxymethyl inulin (CMI). Zinc oxide (ZnO) were synthesized by homogeneous precipitation method and were characterized by SEM, X-ray diffraction analysis, BET and zeta sizer. The effects of the latex particles and green polymer on the crystal growth, morphology and crystalline structure of the resulting zinc oxide were studied by SEM, X-ray diffraction analysis, BET and zeta sizer. The additives affect the dimension, morphology and particle size distribution of the crystals. The reduction in size is greater in the direction of the c-axis. The SEM micrograph shows the formation of well-crystallized, agglomerated small particles of ZnO . The mean size of the subunit determined by XRD is smaller than that of the surface of the grain observed in SEM. The porous ZnO were mainly manufactured by removal of the additives via heat treatment. The additive concentration, sintering time and sintering temperature were varied to investigate their influence on the quality of the porous matrix.

[1] Meldrum, F.C., and Cölfen, H., *Chem. Rev.* **2008**, 108, 4332–4432. [2] Oliveira, A.P.A., Hocheplid, J.P., Grillon, F., Berger, M.H., *Chem. Mater.* **2003**, 15, 3202-3207. [3] Öner, M., Norwig, J., Meyer, W.H., Wegner, G., *Chem. Mater.*, 10(2), 460-463, **1998**. [4] Munoz-Espi, R., Chandra, A., Wegner, G., *Crystal Growth*

& Design, 7, 9, **2007**, 1584–1589. [5] Taubert A., Wegner G., *J. Mater. Chem.*, **2002**, 12, 805–807. [6] Garcia, SP., and Semancik S., *Chem. Mater.* **2007**, 19, 4016-4022.

Keywords: zinc compounds; crystallization; biopolymers

FA2-MS02-P12

Synthetic Dimetaborates $REEAl_{1.67+0.67x}(B_4O_{10})O_x$ ($x \leq 1$) ($REE = \text{La, Ce, Nd, Pm, Sm, Eu}$): Crystal-Chemical Study and Comparison with Natural Counterpart Pepprosiite-(Ce). Francesco Capitelli^a, Nikolay I. Leonyuk^b. ^a*Institute of Crystallography-CNR, Roma, Italy*, ^b*Faculty of Geology, Moscow State University, Moscow, Russia.*

E-mail: francesco.capitelli@ic.cnr.it

In the present work we relate a crystal chemical study of a series of synthetic dimetaborates with composition $REEAl_{1.67+0.67x}(B_4O_{10})O_x$ ($x \leq 1$) [1] ($REE = \text{La, Ce, Nd, Pm, Sm, Eu}$) performed by single-crystal X ray diffraction. The samples were obtained by slow cooling from $\text{K}_2\text{Mo}_3\text{O}_{10}$ based fluxed melts in the form of transparent hexagonal sheet-like crystals. Structure refinements showed all the phases to be isostructural within hexagonal space group $P-62m$ with mineral pepprosiite-(Ce) ($a = 4.612(1) \text{ \AA}$; $c = 9.374(3) \text{ \AA}$ and $V = 172.6 \text{ \AA}^3$) [2], a late pegmatitic - hydrothermal phase from holocrystalline ejecta of the Vico volcanic complex (Italy). The REE cations present a trigonal prismatic coordination; Al cations are surrounded by five oxygen atoms, resembling a square pyramidal coordination, BO_4 groups display tetrahedral arrangement. The three-dimensional framework can be described as a packing of $REEO_6$, BO_4 and AlO_5 polyhedral layers perpendicularly to the crystallographic c axis, held together by strong $REE \dots O$ and $\text{Al} \dots O$ interactions.

[1] Callegari A., Caucia F., Mazzi F., Oberti, Ottolini L., Ungaretti L. *American Mineralogist*, **2000**, 85, 586. [2] Pushcharovskii D.Y., Karpov O. G., Leonyuk N. I., Belov N. V. *Doklady Akademii Nauk SSSR*, **1978**, 241, 91.

Keywords: dimetaborates; rare earth elements (REE); pepprosiite-(Ce)

FA2-MS02-P13

Influence of F^-/OH^- Exchange on the Morphology of Apatite-Gelatine-Composites. Yigit Öztan^a, Paul Simon^a, Rüdiger Kniep^a. ^a*Max Planck Institute for Chemical Physics of Solids. Dresden, Germany.*

E-mail: oeztan@cpfs.mpg.de

Biomimetic apatite-gelatine nanocomposites are grown in a double diffusion setup, where calcium chloride and disodium hydrogen phosphate / sodium fluoride stock solutions diffuse through a gelatine gel from opposite ends under controlled temperature conditions. Composite aggregates are found in periodic growth zones within the gel (Liesegang Bands) and exhibit a hierarchical resemblance to apatite-collagen system found in bone and teeth [1].

The morphology of fluorapatite-gelatine nanocomposites follows a fractal growth mechanism, in which elongated hexagonal seed units first develop into dumb-bell shaped aggregates and ending in notched spheres.

In order to investigate the dependence of the morphology of the aggregates on the initial fluoride amount, a series of experiments was performed where the fluoride concentration was varied and calcium / phosphate concentrations were kept constant (Ca:P:F = 5:3:x, $0.46 < x < 1$). The apatite-gelatine nanocomposites were investigated by means of SEM for their morphology and by X-ray powder diffraction for their crystal structure. While the aggregates preserved the fractal growth mechanism with decreasing fluoride content, a significant change in the morphology of the particles was observed. In fluoride deficient aggregates, the hexagonal seed crystals and the outgrowing branches (Fig. 1), which show self-similarity to the hexagonal seed, became less dense with the subunits exhibiting different thicknesses compared to fluoride-rich aggregates [1]. Decrease in the amount of fluoride was also followed by their X-ray powder diffraction patterns, in which a shift in 2θ to smaller angles was observed indicating an increase in lattice parameters via substitution of hydroxide ions by fluoride ions. Further experiments to investigate the microstructure and the organization of organic fibrils within the composite by means of FIB/TEM, and the chemical composition by means of chemical analyses are in progress. Although similar experiments were reported in literature [2], a fractal morphogenesis of apatite-gelatine aggregates is observed for the first time.

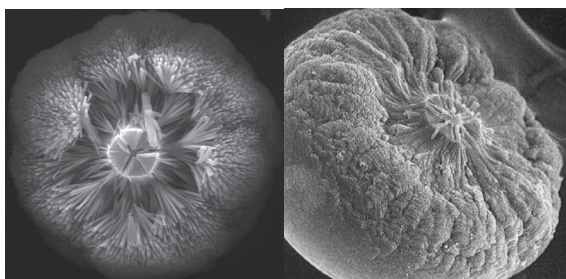


Figure 1. SEM images of broken dumbbells of a) fluoride deficient b) fluoride rich apatite-gelatine composite aggregates. Scale bar $10\mu\text{m}$.

[1] Kniep R., Simon P., *Top. Curr. Chem.*, **2007**, 270, 73-125.

[2] Göbel C., Simon P., Buder J., Tlatlik H., Kniep R., *J. Mater. Chem.*, **2004**, 14, 2225

Keywords: biomineralization; apatite; gelatine composite

FA2-MS02-P14

Crystal Structure of ZnWO_4 (sanmartinite) Scintillator Material in the Range of 3–1423 K. Dmytro M. Trots^a, Anatoliy Senyshyn^b, Leonid Vasylechko^c. ^aHASYLAB at DESY, Notkestr. 85, 22607 Hamburg, Germany. ^bTechnische Universität Darmstadt, FB Material- und Geowissenschaften, Fachgebiet Strukturforchung, Petersenstr. 23, D-64287 Darmstadt, Germany. ^cLviv Polytechnic

National University, Bandera St. 12, 79013 Lviv, Ukraine.

E-mail: dmytro.trots@desy.de; Anatoliy.Senyshyn@frm2.tum.de

The continuous interest in zinc tungstate (sanmartinite) arises from its good scintillation properties. Recent interest in ZnWO_4 is motivated by its excellent prospect in experimental searches for rare events. Since a cryogenic detector has to be cooled down to very low temperatures, information about the thermal expansion of ZnWO_4 is crucial with respect to the thermo-mechanical compatibility with other components of the detector.

Structure of ZnWO_4 (wolframite structure type at room temperature, $P2/c$) was investigated over range of 3–1423 K using synchrotron (B2@HASYLAB [1]) and neutron powder diffraction (SPODI@FRMII [2]). No phase transitions were detected up to the melting point. The low temperature evolution of the ZnWO_4 lattice volume can be modelled fairly well in framework of the 1st order Gruneisen approximation with a Debye approximation for the internal energy [3]. Despite the simplicity of this parameterization, implying a temperature-invariant γ and K , the Debye temperature (370(6) K) and the bulk modulus (161(3) GPa) estimated from this description of the lattice expansion agree well within reasonable limits with the literature values, thus giving strong support for the suitability of the model for ZnWO_4 [3].

The anisotropy of the low temperature thermal expansion is apparent for ZnWO_4 . Equality of $\alpha_{11}(T)$ and $\alpha_{22}(T)$ is readily attributed to the features of the ZnWO_4 structure: each chain of ZnO_6 octahedra is corner-linked in the x - y plane to four chains of WO_6 octahedra and *vice versa*, *i.e.*, the isotropic expansion in the x - y plane can be explained by equivalent corner linkages between rigid octahedral units in the $\langle 110 \rangle$ directions. The expansion along the c -axis – the direction where zigzag chains are formed by either edge-sharing ZnO_6 or edge-sharing WO_6 octahedra – is lower than along the a - and b - directions. The minimum of expansivity corresponds to the direction where more rigid edge-sharing linkages of ZnO_6 or WO_6 octahedra occur. Thus, it is demonstrated how the pronounced anisotropic behaviour in the expansivity of ZnWO_4 can be attributed to the specific structural features [3].

[1] Knapp, M. et al. *J. Synchrotron. Radiat.*, **2004**, 11, 328. [2] Hoelzel, M. et al. *Neutron News*, **2007**, 18, 23. [3] Trots, D. et al. Submitted to *J. Phys.: Condens. Mat.*

Keywords: scintillator materials; crystal structure; thermal expansion

FA2-MS02-P15

Synthesis and Characterization of New Fluorbritholites. A. Hassine^a, N. Jaba^b, K. Bouzouita^a.

^aU. R. Matériaux Inorganiques, Institut Préparatoire aux Etudes d'Ingénieurs, Rue Ibn ElJazzar, 5019 Monastir, Tunisie. ^bDépartement de Physique, Faculté des Sciences de Monastir, 5019 Monastir, Tunisie.

Email: amelhassine@yahoo.fr