

**MS35 P1**

**The Effects of Polyelectrolytes on the Crystallization of Calcium Oxalate Monohydrate** Emel Akyol, Özlem Doğan, Bora Akin, Semra Kirboğa, Mualla Öner  
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**Keywords:** biomineralization, calcium oxalate monohydrate, crystallization.

Biomineralization is the process by which organisms form minerals and is important in many biological events ranging from bone and tooth formation and resorption to pathological mineralization such as renal stone formation and salivary stone formation(1). The application of biomineralization mechanisms allows the controlled growth of crystal with different properties(2-3). On the aspect of biomineralization, it is of interest to study the crystallization of calcium oxalate monohydrate (COM), because COM crystals have been known as a possible source of urinary and kidney stones(4-5). Previous works have shown that the significant influence of urinary macromolecules on calcium oxalate crystallization(6). In this work, we prepared polyelectrolytes with different architectures to explore their relative effectiveness in inhibiting crystal growth of calcium oxalate. Our studies indicate that polyelectrolytes inhibit calcium oxalate monohydrate nuclei so that they are capable of increasing spontaneous nucleation.

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**MS35 P02**

**Structural description of monoclinic Al and Mg-bearing tricalcium silicate.** Miguel A. G. Aranda, Ruth N. de Vera, Ángeles G. de la Torre, *Dept. Química Inorgánica, University of Málaga, Spain*.  
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**Keywords:**  $\text{Ca}_3\text{SiO}_5$ , structural description, Rietveld quantitative phase analysis.

$\text{Ca}_3\text{SiO}_5$  ( $\text{C}_3\text{S}$  in cement nomenclature) is the main constituent of ordinary Portland cements (OPCs). Stoichiometric  $\text{Ca}_3\text{SiO}_5$  exhibits seven polymorphs when heated: three triclinics ( $T_1$ ,  $T_2$ ,  $T_3$ ), three monoclinics ( $M_1$ ,  $M_2$ ,  $M_3$ ) and one rhombohedral (R). However, the presence of foreign ions in the structure may stabilize at room temperature some of the high temperature polymorphs. Monoclinic ( $M_1$  and/or  $M_3$ )  $\text{C}_3\text{S}$  is the polymorph present in OPCs. It usually contains magnesium and aluminium.

In order to perform accurate Rietveld quantitative phase analyses, it is essential to know the best possible structural descriptions of  $\text{C}_3\text{S}$  polymorphs. A crystallographic description for the  $M_3$  superstructure has been reported [1]. However, up to date, there is only a substructure published for  $M_1$   $\text{C}_3\text{S}$  [2].

Four Al and Mg doped  $\text{C}_3\text{S}$  has been synthesized and studied, with nominal formula  $(\text{Ca}_{3-x-z}\text{Mg}_x\text{Al}_z)(\text{Si}_{1-z}\text{Al}_z)\text{O}_5$  with i)  $x=0.03$  and  $z=0.01$ , ii)  $x=0.03$  and  $z=0.02$ , iii)  $x=0.05$  and  $z=0.01$  and iv)  $x=0.06$  and  $z=0.02$ .

We have used neutron and  $\text{CuK}\alpha_1$  strictly monochromatic X-ray powder diffraction data in order to obtain a description of the superstructure of  $M_1$ , with the final goal of improving the phase analyses of Portland cements and clinkers.

We have also prepared some laboratory clinkers with different amounts of Mg, Al and sulphur. Synchrotron X-ray powder diffraction data are used to perform quantitative phase analyses using the  $M_1$  and/or  $M_3$  structural descriptions for  $\text{C}_3\text{S}$ . The implications of the  $\text{C}_3\text{S}$  structure used to model the patterns, as a function of the clinker elemental composition, will be discussed.

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**MS35 P03**

**Formation of In-Sn-phase from ITO-nanoparticles under reducing conditions and its influence on the electrical properties** Gerrit Guenther<sup>a</sup>, Gabi Schierming<sup>a</sup>, Ralf Theissmann<sup>a</sup>, Robert Kruk<sup>a</sup>, Carsten Baehz<sup>b</sup>, Anna Prodi-Schwab<sup>c</sup>, Roland Schmechel<sup>a</sup>, <sup>a</sup>*Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany.* <sup>b</sup>*HASYLAB at DESY, Hamburg, Germany.* <sup>c</sup>*Degussa Cravis GmbH, Marl, Germany.* E-mail: [Gerrit.Guenther@gmail.com](mailto:Gerrit.Guenther@gmail.com)

**Keywords:** transparent conducting oxides, metal phase formation, nanoparticles

Tin doped indium oxide (ITO) is both, electrically conducting as well as optically transparent for wavelengths of visible light. Therefore it is used as a transparent, conducting electrode in numerous electro-optical devices. Pure indium oxide ( $\text{In}_2\text{O}_3$ ) crystallizes as a large unit cell in the so called bixbyite structure (I a -3). The 16c position in this structure is an unoccupied site which is prone to be occupied by further oxygen anions thus creating defects. Doping strongly magnifies this defect and leads to the formation of tin-oxygen clusters which bind conduction electrons [1]. Independent of the deposition method post-deposition-treatments are conducted in reducing gas or technical vacuum at temperatures around 350 °C. The electrical conductivity of ITO-thin films is hereby drastically increased. This is a well known fact which is commonly explained by the selective removal of defect oxygen at the 16c site. Consequently the number of tin-oxygen clusters decreases and less conduction electrons are being bound. Different, more strongly reducing conditions can exceed the removal of defect oxygen and even generate considerable amounts of metallic indium [2].

This motivated the present work which aims at investigating structural changes and at detecting traces of metallic indium in samples that have undergone a temperature treatment in reducing conditions. The samples consisted of spherical, monocrystalline ITO-nanoparticles with a huge surface to volume ratio. In situ synchrotron-XRD measurements were conducted alternately in argon-, oxygen- and hydrogen-gas at temperatures between 25°C and 650°C in order to validate the theory of oxygen-defects. As detection method for metallic indium ex situ susceptibility measurements with a superconducting

quantum interference device (SQUID) were carried out with reduced nano-powders. They were kept under inert conditions after preparation. Complementary transmission electron microscope (TEM) studies of the same samples gave insights into the morphological appearance of the metallic phase.

The results confirm the existence of interstitial oxygen. Additionally the formation of an In-Sn-phase (I 4/mmm) was shown, even under weakly reducing conditions. Due to the liquid state of indium and tin at the process-temperature the interfacial tension leads to the formation of In-Sn balls when the phase-proportion becomes bigger. The balls have a size of 100-800 nm and encase the original ITO-nanoparticles. Furthermore particle growth and surface diffusion are increased in reducing atmosphere. The low electrical resistance of a metallic surface state [3] in combination with the removal of interstitial oxygen could explain the drastic increase of conductivity after reduction treatments.

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#### MS35 P04

**Paramagnetic centers in quartz of basic industry deposits** Yevgeniya Kotova, *Institute of geology, Syktyvkar, Russia*. E-mail: [enkotova@geo.komisc.ru](mailto:enkotova@geo.komisc.ru)

**Keywords:** mineralogy, spectroscopy, quartz.

Quartz is prevailing mineral species and is strategically important mineral raw materials. However pure differences of quartz suitable for synthesis of monocrystals and glass melting used in optics, electronics and other hi-tech industries are enough rare. Hydrothermal and pegmatite deposits of high-quality quartz are known in Russia, the USA, Brazil, Madagascar, China and some other countries.

One of the major quality parameters of quartz raw material for a glass melting is the contents of structural impurities, which determining a limit of quartz raw material washability. The electron spin resonance (ESR) is an effective method for determination some impurity elements in minerals. The main task of the research is estimation and comparative analysis of the contents of the structural impurity-related paramagnetic centers in basic industrial and potentially industrial quartz types of Urals, Kareliya, Eastern Siberia, the USA, China and some other deposits and areas. This investigation is of interest as for the analysis of mineralogenesis conditions as for an estimation of quartz raw materials quality. Researches were made using ESR data on defects connected with isomorphous incorporation of Al- and Ge- ions into the lattice of vein quartz. ESR spectra of Al- and Ge-centres of the powder preparations of quartz were recorded with the radiospectrometer SE/X 2547 (RadioPAN, Poland) at 77 K and 300 K.

The carried out research has shown significant variety of the paramagnetic centers contents in quartz of hydrothermal veins, pegmatites and quartzites. The lowest contents of Al- and Ge-centres are established in the granulated quartz of Subpolar Urals and in quartz from white granites and East Sayan quartzites. It is representing the great interest relative to a problem of high quality quartz raw material for a glass melting.

The increase of average values and of variations ranges of paramagnetic centers concentrations from earlier primarily fine-grained vein quartz generation to later smoky and smoky-citrine quartz generations is stated by the example of Subpolar Urals quartz.

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#### MS35 P05

**The Formation of Nano Hydroxyapatite By Using Polymeric Additives** Özlem Doğan, Emel Akyol, Umut Uysal, Mualla Öner *Yıldız Technical University, Chemical Engineering Department, Davutpasa 34210 Istanbul, Turkey*

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The biological synthesis of inorganic solids often yields materials of uniform size, unusual habit, organized texture and defined structure and composition under moderate conditions of supersaturation and temperature. An understanding of biological solid-state interactions would therefore be of immense value in structural biology and medicine (for example, in the pathological mineralization of bones and teeth and formation of kidney stones) in crystal growth, colloidal and solid-state science (as in the prevention of industrial scaling and controlled synthesis of electronic, magnetic and catalytic devices) and in materials and engineering technology (organized composites and ceramic precursors, and the interrelationships between microstructure and mechanical properties). It seems that new chemical synthetic methods can be developed to form materials with highly controlled microstructures if biomineralization processes can be understood and imitated [1, 2].

Hydroxyapatite (HAP,  $\text{Ca}_5(\text{PO}_4)_3\text{OH}$ ) which is the thermodynamically most stable phase of calcium phosphate is a very important biocompatible material. The controlled nucleation and growth of HAP is essential for the study of hard tissues calcification such as bone and tooth and other undesirable cases of pathological mineralization such as articular cartilage and stones in gall bladder and kidney [3, 4].

In general, biominerals are formed by the precipitation of calcium carbonate, calcium phosphate and other minerals within polymeric tissue matrices. It is thought that the organic polymer matrix is the key to the micro structural control. Acidic proteins can be incorporated into mineralizing tissues and are believed to be responsible for both nucleation and inhibition of crystallization [5].

In this work that we investigate HAP crystallization as a model for biomineralization. The constant-composition method has been used to study the individual effect of polymeric additives for the HAP crystallization. The polyvinylphosphonate, bisphosphonate polymers and carboxymethylulin green polymers have been used as additives for controlling crystallization.

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