

MS35 P1

The Effects of Polyelectrolytes on the Crystallization of Calcium Oxalate Monohydrate Emel Akyol, Özlem Doğan, Bora Akin, Semra Kirboğa, Mualla Öner
Yıldız Technical University, Chemical Engineering Department, Davutpasa 34210 Istanbul, Turkey
E-mail: ekyol@yildiz.edu.tr and oner@yildiz.edu.tr

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.

(1)Westbroek P, De Jong EW(eds). *Biomineralization and Biological Metal Accumulation*. D. Reidel Publishing Company: Dordrecht, 1983.

(2) Berman A, Addadi L, Weiner S. *Nature* 1988; 331:546.

(3) Oner M, Norwig J, Meyer WH, Wegner G. *Chem. Mater.* 1998; 10(2):460-463.

(4) Jung T, Kim WS, Choi C.K, *Material Science and Engineering C*, 2004, 24-33.

(5) Akyol E, Bozkurt A, Oner M, *Poly. for Adv.Technol.* 2006; 17:58-65.

(6) Grover PK, Moritz RL, Simpson RJ, Ryall RI. *Eur. J. Biochem.* 1998; 253: 637.

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.*
E-mail: g_aranda@uma.es

Keywords: Ca_3SiO_5 , structural description, Rietveld quantitative phase analysis.

Ca_3SiO_5 (C_3S in cement nomenclature) is the main constituent of ordinary Portland cements (OPCs). Stoichiometric Ca_3SiO_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) C_3S 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 C_3S 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 C_3S [2].

Four Al and Mg doped C_3S 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 C_3S . The implications of the C_3S structure used to model the patterns, as a function of the clinker elemental composition, will be discussed.

[1] De la Torre, A.G., Bruque, S., Campo, J., Aranda, M.A.G., *Cem Concr Res*, 2002, 32, 1347.

[2] De Noirfontaine, M.-N., Dunstetter, F., Courtial, M., Gasecki, G., Signes-Frehel, M., *Cem. Concr. Res*, 2006,36, 54.

MS35 P03

Formation of In-Sn-phase from ITO-nanoparticles under reducing conditions and its influence on the electrical properties Gerrit Guenther^a, Gabi Schierming^a, Ralf Theissmann^a, Robert Kruk^a, Carsten Baehz^b, Anna Prodi-Schwab^c, Roland Schmechel^a, ^a*Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany.* ^b*HASYLAB at DESY, Hamburg, Germany.* ^c*Degussa Cravis GmbH, Marl, Germany.* E-mail: 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 (In_2O_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