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Czech Republic

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Laboratory of Phys. and Chem. Analysis

PhD research projects.

Formulation of amorphous Mg-K phosphate ceramics for bioengineering applications.

<u>Scientific Background</u>

Magnesium-potassium phosphate ceramics are chemically-bonded ceramics [1]. Their properties make them attractive for applications like waste encapsulation, bone repair, natural fibre composites. When MgO reacts with potassium di-hydrogen phosphate (KDP) in solution, formation of K-struvite (MKP) occurs: $MgO + KH_2PO_4 + 5H_2O = MgKPO_4{\bullet}6H_2O$. There are experimental evidences that, besides crystalline MKP, an amorphous phase also forms.

<u>Results of our previous investigations</u>

Over long times, we found that amount of amorphous decreases whereas that of MKP increases, and so do mechanical properties [2,3,4]. Although considered a precursor of crystalline MKP, at the current state of knowledge, the nature of this amorphous phase remains unexplained.

We conducted kinetics synchrotron diffraction experiments [5] on samples with MgO having different specific surface area and reactivity. A mechanism for the reaction has been proposed.

Small angle neutron scattering experiment [4,6] allowed us to show the dependence of microstructure from reactivity of MgO and that the development of the crystalline product during the setting reaction scales with the microstructural parameters.

Quasielastic neutron scattering technique (QENS) and nuclear magnetic resonance (NMR) spectroscopy have been employed and results are under evaluation to describe the amorphous phase and the state of water in the system during the reaction.

<u>Description</u>

Amorphous systems are interesting for bioengineering applications because of their properties such as bioresorption.

I. Formulation of a stable amorphous ceramic material based on Mg and P. Identification of the reagents and optimization of formula.

II. Characterisation of the ceramic material. Prove its composition, link this information to the mechanical properties of the final product. Micro Raman spectroscopy, FTIR/DRIFT spectroscopy, nanoindentation and SEM. Use of PDF analysis with data collected at synchrotron sources and NMR.

III. Elucidate the role of water in the system using QENS. Different contributions, describing populations which contain water with different degrees of confinement can be detected. Thus, QENS provides a direct measure of the conversion of free water into structurally/chemically bound water, and into water constrained/confined in the pores of the paste.

IV. Study of adhesive properties with metals and bone materials. Spectroscopic techniques (micro-Raman, FTIR, XPS, Auger electron spectroscopy)

During the proposed plans of activities, the student will greatly improve his/her scientific background becoming familiar with several analytical techniques (some of them highly advanced) for the study of the properties of materials; he/her will take advantage of the possibility of performing experiments both in the laboratory and at international large scale facilities and get in contact with international scientific environments. This expertise could be useful for the development of his/her career in both private and academic research contexts.

Profile requested: dynamic individuals, enthusiastic about science with a background in materials science, preferably chemistry/chemical engineering but not limited to them, interested in doing experimental work and elaborate results according to theories.

Alberto Viani

References

[1] Wagh AS. Magnesium phosphate ceramics, in: E. Hurst, editor. Chemically bonded phosphate ceramics: 21st century materials with diverse applications, Elsevier, Amsterdam, 2004.

[2] A. Viani and A. F. Gualtieri, Preparation of magnesium phosphate cement by recycling the product of thermal transformation of asbestos containing wastes, Cem. Concr. Res., 58 (2014) 56-66.

[3] M. Pérez-Estébanez, P. Mácová, P. Sasek, A. Viani and A. Gualtieri, Mg-phosphate ceramics produced from the product of thermal transformation of cement-asbestos, J. Polish Miner. Eng. Society, 187 (2014).

[4] Viani, A., Sotiriadis, K., Šašek, P., & Appavou, M. S. (2016). Evolution of microstructure and performance in magnesium potassium phosphate ceramics: Role of sintering temperature of MgO powder. *Ceramics International*, *42*(14), 16310-16316.

[5] A. Viani, M. Pérez-Estébanez, S. Pollastri, A.F. Gualtieri In situ synchrotron powder diffraction study of the kinetics of setting of magnesium-potassium phosphate ceramics: influence of MgO reactivity. Cem. Concr. Res., (2016) DOI:10.1016/j.cemconres.2015.10.007

[6]A. Viani, A. Radulescu, M. Pérez-Estébanez. Characterisation and development of fine porosity in magnesium potassium phosphate ceramics. Materials Letters, 161, 628-630 (2015).