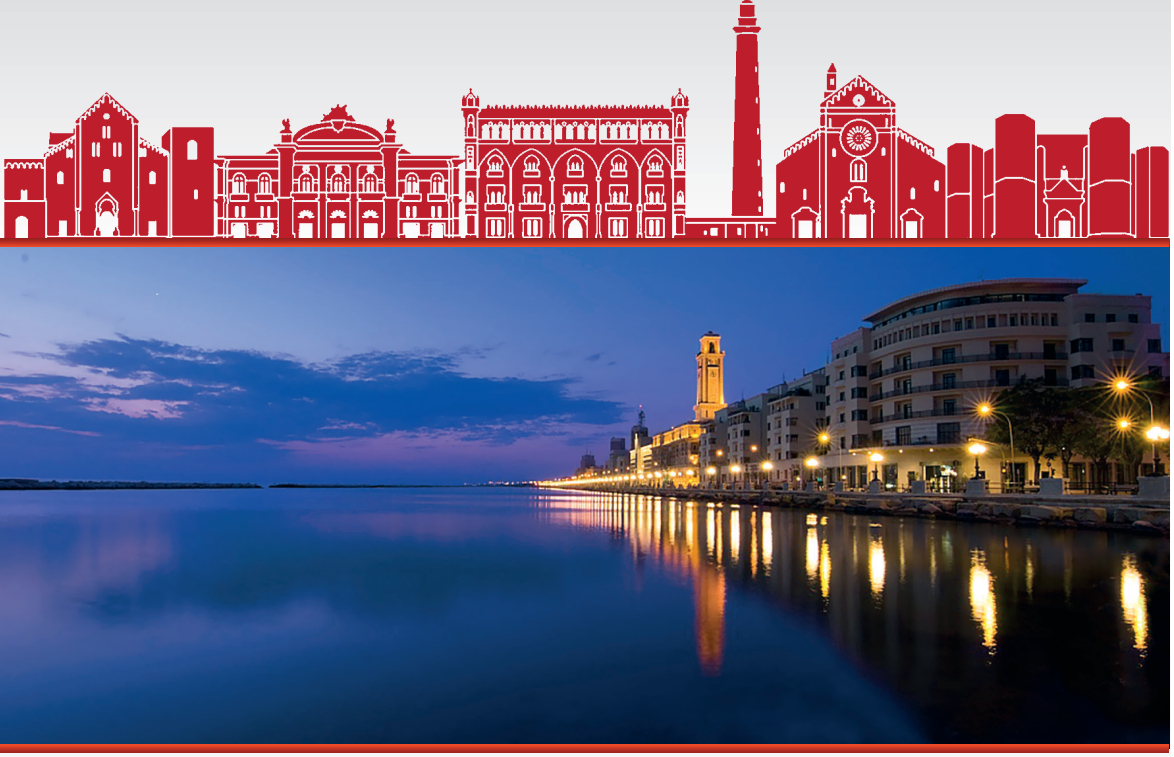

EPDIC 15

The European Powder Diffraction Conference

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BOOK OF ABSTRACTS

EPDIC15

[1] H. Sowa, H. Ahsbahs *Acta Cryst*., 1998, B54, 578. [2] S. K. Wolff, D. J. Grimwood, J. J. McKinnon, M. J. Turner, D. Jayatilaka, M. A. Spackman, CrystalExplorer 3.0, University of Western Australia, 2012.

Keywords: high-pressure diffraction, compression mechanism

MS12-P03 Applications of synchrotron x-ray powder diffraction in hydrated cements: high-resolution and high-pressure studies

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The main aim of this study is to apply synchrotron radiation techniques for the study of hydrated cement pastes. In particular, the tetracalcium aluminoferrite phase, C_4AF in cement nomenclature, is the major iron-containing phase in Ordinary Portland Cement (OPC) and in iron rich belite calcium sulfoaluminate cements.
In a first study, the hydration mechanism of pure tetracalcium aluminoferrite phase with water-to-solid ratio of 1.0 has been investigated by HR-SXRPD (high resolution synchrotron X-ray powder diffraction). C_4AF in the presence of water hydrates to form mainly an iron-containing hydrogarnet-type (katoite) phase, $C_3A_{0.84}F_{0.16}H_6$, as single crystalline phase. Its crystal structure and stoichiometry were determined by the Rietveld method and the final disagreement factors were R_{WP}=8.1% and R_F=4.8% [1]. As the iron content in the product is lower than that in C_4AF, it is assumed that part of the iron also goes to an amorphous iron rich gel, like the hydrated alumina-type gel, as hydration proceeds. Further results from the high-resolution study will be discussed.
In a second study, the behavior of pure and iron-containing katoites (C_3AH_6 and $C_3A_{0.84}F_{0.16}H_6$) under pressure have been analyzed by SXRPD using a diamond anvil cell (DAC) and then their bulk moduli were determined. The role of the pressure transmitting medium (PTM) has also been studied. In this case, silicone oil as well as methanol/ethanol mixtures have been used as PTM. Some "new peaks" were detected in the pattern for $C_3A_{0.84}F_{0.16}H_6$ as pressure increases, when using ethanol/methanol as PTM. These new peaks were still present at ambient pressure after releasing the applied pressure. They may correspond to crystalline nordstrandite or doyleite from the crystallization of amorphous aluminium hydroxide. The results from the high-pressure study will also be discussed.

[1] Cuesta A., Santacruz I., Sanfélix S.G., Fauth F., Aranda M.A.G. and De la Torre A.G. *Constr Build Mater*, 2015, 101, 818.

Keywords: Synchrotron radiation, hydrated cements, high-pressure, bulk moduli

MS12-P04 Mechanical Properties of the isostructural Gallium and Aluminum Fumarate Metal-Organic Frameworks: A Joint Experimental-Modelling Exploration

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Metal–organic frameworks (MOFs) are a relatively new class of hybrid materials consisting of crystalline networks formed by metal ions or metal clusters connected *via* organic ligands. Their porous frameworks exhibit a wide range of properties of great promises for diverse societally relevant applications in the fields of environment, energy and biomedicine [1]. In this context, there have been very few studies on the thermo-mechanical properties of MOFs [2]. Recently, we showed that the commercialized Aluminium Fumarate MOF, MIL53(Al)-FA, undergoes a reversible structural contraction under an applied pressure above 100MPa, with an associated work energy of 60 $J.g^{-1}$, which is among the highest values reported for porous solids [3]. As part of our ongoing investigations into related flexible,

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