

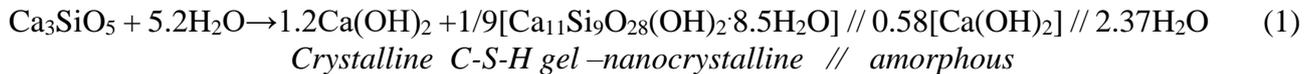
## Pair distribution function as a tool to characterize C-S-H gels

A. Cuesta, A. Morales-Cantero, A.G. De la Torre, I. Santacruz, M.A.G. Aranda

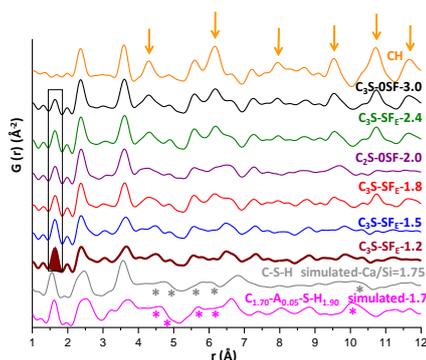
Departamento de Química Inorgánica, Universidad de Málaga, 29071-Málaga (Spain)

a\_cuesta@uma.es

Portland cement (PC) is the most manufactured product in the world. However, cement industry is one of the major contributors for greenhouse gas emissions. For every ton of grey PC clinker, around 0.87 CO<sub>2</sub> tons are released into the atmosphere. For this reason, alternative cements having similar performances to ordinary PC are needed. A recent work [1] has identified the use of supplementary cementitious materials (SCMs) as the most favourable approach for lowering CO<sub>2</sub> emissions in the cement industry. The hydration reactions of tricalcium silicate, Ca<sub>3</sub>SiO<sub>5</sub> (main phase of PC) consist of its dissolution, the precipitation of the nanocrystalline C-S-H gel, jointly with the formation of portlandite, Ca(OH)<sub>2</sub> according to equation (1). C-S-H gel was described to be composed by defective nanocrystalline clinotobermorite, amorphous Ca(OH)<sub>2</sub> and gel pore water [2]. The calcium hydroxide formed in reaction (1) can be employed to yield additional secondary C-(A)-S-H through the pozzolanic reaction with SCMs.



The analysis of nanocrystalline/amorphous phases in cement matrices which contain high amounts of crystalline phases is very challenging. Pair distribution function (PDF) in combination with synchrotron radiation is key to characterize cement pastes. This work focuses on the characterization of amorphous and nanocrystalline phases which are present in cement related pastes by total scattering PDF. We have studied a series of tricalcium silicate pastes blended with silica fume hydrated at four months and dicalcium silicate pastes hydrated at longer ages [3]. PDF data were collected at ALBA Synchrotron, beamline MSPD, see Figure 1. The changes in the local atomic order of the C-S-H gels formed from the hydration of pastes with silica fume by varying the overall Ca/Si ratio were followed. It was found that the C-S-H gel formed by the pozzolanic reaction showed nearly the same local structure than the primary C-S-H gel from equation (1).



**Figure 1.** Synchrotron PDF patterns for the tricalcium silicate blended with silica fume pastes and dicalcium silicate paste. The experimental plot for commercial portlandite and the theoretical PDF patterns for C-S-H and C-S-(A)-H are given as references [3].

- [1] UN Environment, et al. (2018), Eco-efficient cements: Potential, economically viable solutions for a low-CO<sub>2</sub>, cement-based materials industry, *Cem. Concr. Res.* **114**, 2–26.
- [2] Cuesta, A., et al. (2018), Multiscale understanding of tricalcium silicate hydration reactions, *Sci. Rep.* **8**, 8544.
- [3] Cuesta, A., et al. (2021), Local structure and Ca/Si ratio in C-S-H gels from hydration of blends of tricalcium silicate and silica fume, *Cem. Concr. Res.* **143**, 106405.

*This research was funded by Ministry of Science (Spain), grant number PID2019-104378RJ-I00*