Synchrotron X-ray pair distribution function analysis of calcium silicate pastes

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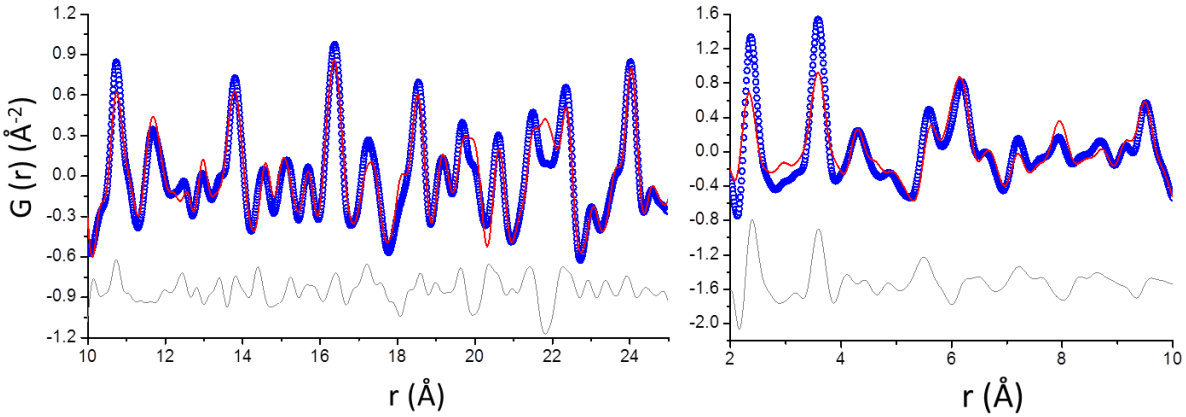
The analysis of nanocrystalline and amorphous phases in cement matrices which contain high amounts of crystalline phases is a very challenging task. In this respect, pair distribution function (PDF) methodology in combination with synchrotron radiation is very useful to characterize cement pastes. PDF data can give insight about the atomic local structure of the non-crystalline components such as C-(A)-S-H gels. This work is focused on the characterization of amorphous and nanocrystalline gels which are present in cement related pastes by total scattering PDF analyses in selected samples. In addition, the PDF approach also allows us to perform quantitative analysis in order to know the nanocrystalline and microcrystalline contents. [1]

X-ray scattering data of different pastes were collected in BL04-MSPD beamline at ALBA Synchrotron (Barcelona, Spain). Three sets of hydrated samples have been studied and they will be reported: (i) tricalcium silicate, Ca_3SiO_5, the main component of Portland cements; (ii) dicalcium silicate, Ca_2SiO_4, the main component of belite cements; and (iii) tricalcium silicate samples mixed with different amounts of silica fume (as the simplest example of supplementary cementitious materials). For all the PDF analyses, a multi r-range approach was followed (see Figure below): the higher r-range (e.g. 40-80 Å) is used to determine the microcrystalline phase contents, for instance, portlandite and anhydrous phases; then, the intermedium r-range allows characterizing the atomic ordering in the nanocrystalline fraction of the C-S-H gel (e.g. 10-40 Å); and finally, the low r-range, below ≈10 Å, gives information about the chemical nature of the additional amorphous components [2].



Literature:
[1] Cuesta, A.,et al. (2017). Aluminum hydroxide gel characterization within a calcium aluminate cement paste by combined Pair Distribution Function and Rietveld analyses. Cement and Concrete Research, 96, 1-12.
[2] Cuesta, A, et al (2018). Multiscale understanding of tricalcium silicate hydration reactions. Scientific Reports, 8, 1, 8544.