PAIR DISTRIBUTION FUNCTION STUDIES IN CEMENTITIOUS SYSTEMS

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The analysis of amorphous/nanocrystalline phase(s) within cement matrices that contain high amounts of crystalline phase(s) is very challenging. Synchrotron techniques can be very useful to characterize such complex samples.[1] This work is focused on total scattering Pair Distribution Function (PDF) quantitative phase analyses in selected real-space ranges for a better understanding of the binding gel(s). Powder diffraction data collected in BL04-MSPD beamline have been analyzed by PDF and Rietveld methodologies to determine nanocrystalline and microcrystalline phase contents. The comparison between both methodologies allows us to have a better insight about the nanocrystalline/microcrystalline components which coexist in cement pastes. Three sets of hydrated model samples have been studied: i) monocalcium aluminate, $CaAl_2O_4$, the main component of calcium aluminate cements, ii) ye'elimite, $Ca_4Al_6SO_{16}$, the main component of calcium sulfoaluminate cements, and iii) tricalcium silicate, Ca_3SiO_5, the main component of Portland cements.

For the $CaAl_2O_4$ paste, the PDF fit shows that the aluminum hydroxide gel has a gibbsite local structure with an average particle size close to 5 nm.[2] Figure 1 shows the final fit for $CaAl_2O_4$ paste in two different real-space regions. On the contrary, for $Ca_4Al_6SO_{16}$ paste, it has been found that the particle size of the aluminum hydroxide gel is below 3 nm. Moreover, the Ca_3SiO_5 paste contains a different nanocrystalline gel, C-S-H, which has also been thoroughly studied. Different crystal structures (including Tobermorite, Clinotobermorite and Jennite) have been tested to find the structural model that fits better the experimental data. The results from this ongoing investigation will be reported and discussed.

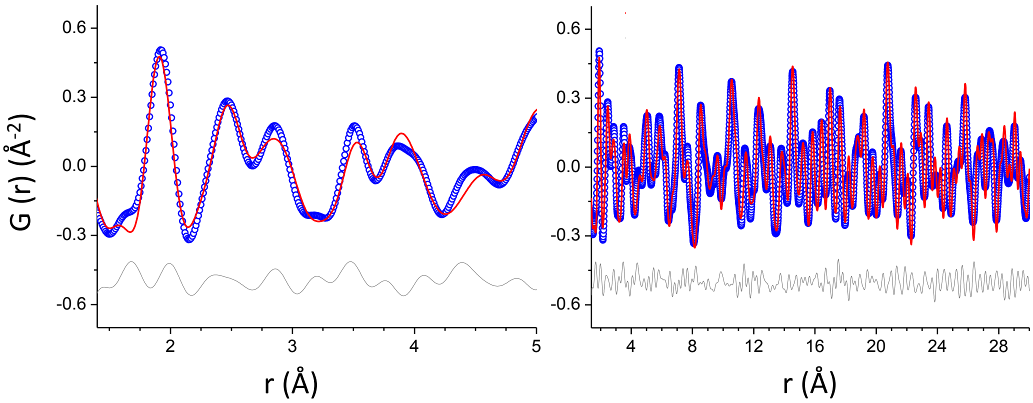

Figure 1. Experimental (blue circles) and fitted (red solid line) PDFs for $Ca_2Al_4O_4$ paste at selected ranges.

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[1] M.A.G. Aranda, *Cryst. Rev.* **2016**, *22*, 150-196.
[2] A. Cuesta, et al., *Cem. Concr. Res.* **2017**, *96*, 1–12.