Thermal and chemical stability of calcium-silicate-hydrate gel

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Calcium-silicate-hydrate (C-S-H) gel is the main binder component in ordinary Portland cement (OPC)-based concrete, and therefore the long-term durability of this ubiquitous construction material is partially controlled by the stability of the C-S-H gel. However, due to the disordered nature of this gel phase at the atomic and nanoscale, it is extremely difficult to accurately pin-point the effects various degradation environments have on the gel. Here, the atomic structure of C-S-H gel is experimentally investigated using X-ray and neutron total scattering and pair distribution function (PDF) analysis, specifically to discover the structural changes induced due to exposure to certain thermal and chemical environments.

When C-S-H gel is exposed to elevated temperatures, it is known that there is densification of the gel and a loss of pore and interlayer water. Here, it will be shown that the type of water being removed from the sample (capillary versus gel pore water) can be pin-pointed using in situ neutron PDF analysis. The results reveal that above a certain temperature all of the pore water is removed from the C-S-H gel, at which stage significant changes in the calcium silicate layers are seen in the data due to the additional loss of interlayer water molecules and reorganization of the anhydrous phase.

PDF analysis has also been used to investigate the impact of carbon dioxide molecules on the structure of C-S-H gel. Here, in situ X-ray PDFs of the carbonation of C-S-H gel will be presented, including results on the atomic structure of the decalcifying gel and associated reaction kinetics. It will be shown that the results reveal important new information on the atomic structure of the amorphous silica gel, including the presence of residual calcium in the gel, possibly in the form of amorphous calcium carbonate.