Influence of amino acids on the crystallization of calcium silicates hydrates

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The hydration of Portland cement lead to Calcium silicate hydrates which are prominent for their high mechanical strength. Cement clinker production causes up to 7 % to the global CO2-emissions. One of several strategies in order to reduce this large carbon footprint are the use of supplementary cementing material (SCMs), e.g. natural and artificial puzzolanes[1]. The application of SCM’s possess several disadvantages when it comes to practical application. The, decreased in the evolvement of strength is an unfavourable disadvantage. A promising starting point for an extensive use of SCM’s is the use of approaches of biomineralisation to effect crystal shape and size. Nature provides many examples for materials of high mechanical strength and chemical resistance like shells (Calcium carbonate) diatoms (SiO$_2$) or bones (Calcium phosphates). Calcium silicate hydrates are not known in biomineralization processes. Focusing on the functional groups involved in biomineralisation processes, it can be stated that functionalities like -COOH-, -OH, as well as imidazolium-containing structures and amino acids are involved very often [2].

A model system starting from CaO (Alfa Aesar) with fumed silica (Evonik) in aqueous media was used to synthesize the Calcium silicate hydrate phase Tobermorite. L-Glutamine, L-Alanine, L-Serine, L-Histidine, 6-Aminohexanoic acid, Imidazole and Chitosan and Carboxy methyl chitosan was used to study their influence on the crystallization.

X-ray powder diffraction measurements were performed using a D2-Phaser (Bruker-AXS) diffractometer using CuKa ($\lambda = 0.15406$ nm) radiation and a 1-dimensional Lynxeye PSD detector. Monoclinic 11 Å Tobermorite was used as structural model for all refinements, lattice parameters hereof were used as staring parameters for each refinement cycle [3]. Since detailed information about atomic positions is still lacking, a Pawley fit was performed.

The presence of the amino acids lead in most cases to the enlargement of the unit cell. The a-axes of the unit cell is effected only in presence of Imidazole and 6-aminohexane acid. The b-axes is effected by the addition of Chitosan and Carboxy methyl chitosan. The c-axes increases with addition of the α-amino acids Glutamine, Alanine and Histidin.

Literature