o.m6.o3 **Tricalcium Silicate Ca_3SiO_5: the major compound of anhydrous Portland cement revisited.**
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Tricalcium Silicate Ca_3SiO_5, about 70 %, of anhydrous Portland cement, exhibits a rather complex phase diagram, surprisingly still not well known. With the usual compact stoechiometric notation, C=CaO and S=SiO_2, it is usually refered as C3S. Among the various crystal structures (rhombohedral, monoclinic or triclinic) found in the phase diagram as a function of temperature and impurities, one finds most frequently the two high temperature monoclinic M1 and M3 phases, stabilised at room temperature by impurities.

Powder diffraction is now widely used for an efficient quantification of mixtures. But anhydrous cement usually exhibits at least four distinct compounds with at least two monoclinic compounds with overlapping Bragg lines in the diffractograms. We are also faced with the difficulty to distinguish among the various phases arising from the polymorphism of C3S itself, and therefore to an additional problem of phase identification. To be tractable, the -most widely used- Rietveld analysis, needs either precise and not too difficult atomic models, which is not the case of C3S. The M3 phase is known from single crystal studies, with very complex models involving orientational disorder of silicate tetrehedra, splitted atoms and often superstructures with large unit cells. On the contrary, the only known description of the M1 phase is a short list of intensities, with a five levels scale from very strong to very weak, without any atomic model.

Various compounds, synthetised at the CTG (M3, M2, M1 and T1) have been studied by X-ray powder diffraction with Rietveld analysis. The known results can be modified and unconventional unit cells are found, which make it possible to understand the metric relation between the various phases, from triclinic to rombohedral. Starting from this analysis, a space group and an atomic model can be found for M1 structure. Two small Bragg lines of the M3 phase, related to a propagation vector, are found of special importance to distinguish between the M1 and M3 forms.

Industrial cements are also discussed.

Carrying the discussion further than the usual one, restricted to a more or less complex orientational disorder of a group of three silicate tetrahedra looking like "alone in the space", we introduce various 1-D, 2-D, and 3-D structural units, which make it easier to understand the actual phase diagram. Some keys toward a better understanding of the orientational disorder and the structural effect of impurities on the structure are discussed.

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