ON THE FORMATION OF CEMENTITIOUS C-S-H NANOPARTICLES: A COMPUTATIONAL APPROACH

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Abstract:

Much of the existing knowledge on the nanostructure of cementitious Calcium Silicate Hydrate (C-S-H) nanoparticles has been gained from structural comparisons with crystalline calcium silicate hydrates. In fact, several models [1-5] have been proposed so far that draw structural analogies with tobermorite and jennite crystals and/or with distorted semi-crystalline variations of them (the so called C-S-H (I) and C-S-H (II) phases respectively). From these models, C-S-H gels can be approximately viewed as layered structures, in which calcium oxide sheets are ribbed on either side with silicate chains, and free calcium ions and water molecules are present in the interlayer space (see Figure).

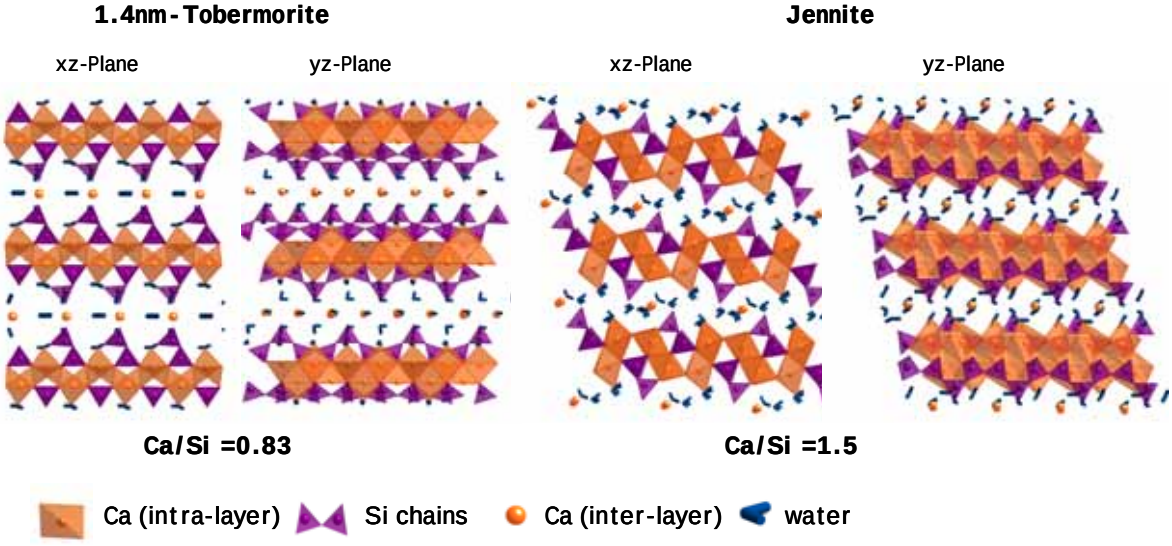

Figure: Schematic representation of the structure of the 1.4-nm tobermorite and jennite crystals.

However, and though intensively characterized by techniques like SEM, TEM, NMR, etc [6], many features of the nanostructure of C-S-H gel remain unravelled. The debate about the short-range ordering of cementitious C-S-H gel is still unsettled.

This work aims to highlight the importance of atomistic computational approaches to shed light on the nanostructure of the C-S-H gels. To this end two complementary ongoing studies will be presented. Firstly, the dependence of the mechanical properties upon the length of the silicate chains will be

discussed with help of force-field calculations [7]. Secondly, the underlying growth mechanisms which govern the formation of C-S-H nanoparticles will be studied by means of *ab-initio* [8] and Molecular Dynamic calculations [9].

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