COMPUTATIONAL STUDY OF THE MECHANICAL PROPERTIES OF TOBERMORITE AND JENNITE CRYSTALS IN COMPARISON WITH C-S-H GEL

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Cement paste matrix is a complex multi-phase, heterogeneous and amorphous material. Among its hydration products, the so called C-S-H (Calcium Silicate Hydrate) gel is the most important one. It is responsible for the hardness and cohesion of the material, and it represents up to the 70% by volume of the cement paste

Yet intensively characterised by techniques such as SEM, TEM, XDR, NMR, etc [1], the complex and poorly organised nanostructure of the C-S-H gel has not been completely elucidated. Nevertheless certain structural features are already recognised. For instance, it is fair to say that, in essence, C-S-H gel is composed of silicate chains held together by calcium oxide layers, as schematically represented in Fig. 1. In fact, several models have been proposed so far which represent the atomic scale of C-S-H gel as a mixture of Tobermorite-like and Jennite-like structures in which these crystalline and layered species show multiple defects and imperfections [2].

At larger scales, let say from 1nm to 100 nm, the exiting descriptions of the C-S-H gel have been centred in the recognition of the colloidal and gel-like properties of the C-S-H gel. The current vision is the so called Jennings model [3], which states that certain basic (almost spherical) building blocks exist, and that they pack themselves to build up the C-S-H structure. According to this model, two kinds of C-S-H gels arise, the high-density (HD) C-S-H gel and low density (LD) C-S-H gel, depending on the packing efficiency of the basic building blocks. Interestingly, both varieties (LD and HD) exhibit dissimilar mechanical properties, as recently shown by nanoindentation experiments [4,5].

Thus, important technological applications in the construction sector are clearly envisaged provided the appearance HD C-S-H gels could be somehow favoured. To this end, it is clear that a closer linkage between the layered morphologies addressed in the structural models and the rounded basic building blocks proposed in Jennings model colloidal is clearly needed.

This work precisely attempts to shed light on this issue from a theoretical viewpoint. By means of ab-initio calculations with SIESTA code [6] and semiempirical calculations with GULP code [7], the mechanical properties of both Tobermorite and Jennite crystals and suggested smaller pieces of them will be assessed and compared with the existing experimental data. Special emphasis will be also paid to the establishment of linkages between the structural and colloidal viewpoints.

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Figures:

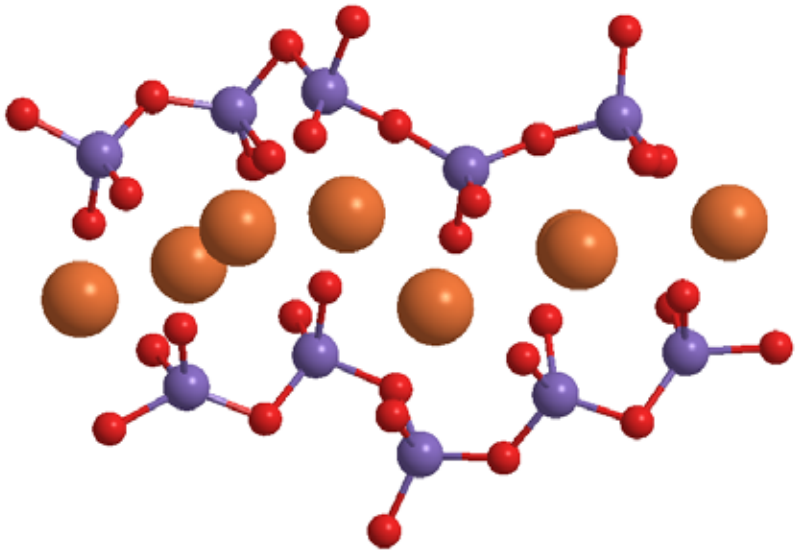

Fig 1. Schematic representation of the C-S-H gel.