MOLECULAR DYNAMIC STUDY OF THE N-A-S-H GEL IN ALKALI-ACTIVATED FLY-ASHES CEMENTS.

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Ordinary Portland Cement (OPC) is one the most employed materials in construction and its importance is beyond any doubt. The main component of the cement paste is the Calcium Silicate Hydrated (C-S-H) gel, which is the principal responsible for the cohesion and hardness of the final cementitious material. This C-S-H gel is an amorphous product, with variable composition, although it has some order at the nanoescale [1, 2]. This variable and amorphous nature implies difficulties in the characterization, and many aspects of the atomic- and nano-structure of the C-S-H gel remain unclear. Fortunately recent atomistic simulations have provided crucial information such as the number of Si-OH and Ca-OH bonds, the length of silicate chains, or degree of polymerization for different Ca/Si ratios [3], and present themselves as a promising tool to shed light on the nanostructure of CSH gels.

Parallel to the OPC, the interest in new types of cement is increasing. The durability, mechanical properties, design and even esthetical requirements for cementitious materaials are increasing continuously. Other important aspects are the sustainability of the manufacture process and wastes recycling. One of the most promising alternatives are the alkali-activated fly-ashes cements. Analogous to the C-S-H gel in OPC, an amorphous reaction product is obtained in the curing process of alkali-activated fly-ashes cements, the N-A-S-H gel. It has a disorder network structure related to that of zeolites, based in silicon-aluminium-sodium and water. The N-A-S-H gel has a similar function to the C-S-H gel, being the main responsible of the properties of the material [4, 5]

The nanostructure of the C-S-H gel has been recently studied by Molecular Dynamics simulations providing useful information. Some important parameters as the number of Si-OH and Ca-OH bonds, length of silicate chains, or degree of polymerization were studied for different Ca/Si ratios [3] finding a reasonable agreement with the experimental evidence. In this work we apply the same scheme to study the nanostructure of N-A-S-H gel. For this purpose, three different samples with different Si/Al ratios (1.5, 1.75 and 2) will be studied by means of Molecular Dynamics simulations, with the Tremolo code [6]. To this end, both important chemical parameters such as the as the number of Si-OH, Al-OH and Na-OH bonds and the connectivity of the (alumino)silicate structures will be analysed.

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