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# Atomic-Level Structure of the Calcium Silicate Hydrate Nanofoil and Adsorption of $Ca^{2+}$

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Concrete is the most manufactured material, and it accounts for 8% of all $CO_2$ emissions. While the bulk structure of the main hydration phase calcium silicate hydrate (C-S-H) is today well understood, the C-S-H surface is still not explored, and somewhat of a mystery. It is known that C-S-H has a high specific surface area (200 - 300 $m^2/g$), which makes it de facto of great importance for concrete properties. The different phases in cement dissolve during hydration to make the solution very complex with several ionic species. There are many unknown interactions at the interface of C-S-H, including sulfate adsorption, additives and chloride binding and transport which cause major durability issues in service life of reinforced concrete structures. To study and understand these phenomena a description of the surface is needed, which should come in the form of a realistic-pragmatic model surface, since C-S-H is poorly nanocrystalline, meaning there will be no long-range order as we observe in crystalline systems.

Recent advances in understanding the atomic structure of C-S-H are due to combined experimental and modeling work. While advanced characterization techniques can help in elucidating the surface termination of particles, they usually cannot be used for C-S-H characterization, due to its complex nanofoil geometry. However, standard techniques such as synchrotron XRD, $^{29}Si$ NMR, RAMAN and IR spectroscopy provide enough information for the definition of a realistic-pragmatic C-S-H surface.

In this work we show how the brick model from Kunhi Mohamed et al. can be used to construct the (001) basal C-S-H surface. A new multiparameter approach in describing the (001) basal C-S-H surface is shown and how the surface termination affects the overall properties (Ca/Si ratio, mean chain length, relative concentration of silanol and hydroxide groups). We argue that the surface is dominantly calcium terminated and we propose a calcium adsorption mechanism, which agrees with previous studies.

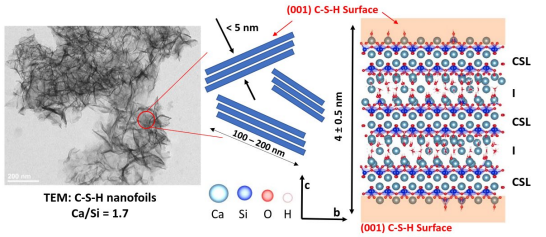


Figure 1. C-S-H nanofoils. Left TEM image of synthetic C-S-H with Ca/Si = 1.7. Right: computational model of 3 layers, 2 interlayers thick C-S-H nanofoil with the dominant (001) basal surfaces. I – interlayer, CSL – calcium-silicate layer