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Carbonation of Wollastonite (001) competing Hydration: Microscopic Insights from Ion Spectroscopy and Density Functional Theory

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Abstract : In this work, we report about the influence of the chemical potential of water on the carbonation reaction of wollastonite (CaSiO3) as model surface of cement and concrete. Total energy calculations based on density functional theory (DFT) combined with kinetic barrier predictions based on nudge elastic band (NEB) method show that the exposure of the water-free wollastonite surface to CO2 results in a barrier-less carbonation. CO2 reacts with the surface oxygen and forms carbonate (CO32-) complexes together with a major reconstruction of the surface. The reaction comes to a standstill after one carbonate monolayer has been formed. In case one water monolayer is covering the wollastonite surface, the carbonation is no more barrier-less, yet ending in a localized monolayer. Covered with multilayers of water, the thermodynamic ground state of the wollastonite completely changes due to a metal-proton exchange reaction (MPER, also called early stage hydration) and Ca2+ ions are partially removed from solid phase into the H2O/wollastonite interface. Mobile Ca2+ react again with CO2 and form carbonate complexes, ending in a delocalized layer. By means of high resolution time-of-flight secondary-ion mass-spectroscopy images (ToF-SIMS), we confirm that hydration can lead to a partially delocalization of Ca2+ ions on wollastonite surfaces. Finally, we evaluate the impact of our model surface results by means of Low Energy Ion Scattering (LEIS) spectroscopy combined with careful discussion about the competing reactions of carbonation vs. hydration.

Keywords : Calcium-silicate, carbonation, hydration, metal-proton exchange reaction

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