A BOTTOM-UP HIERARCHICAL MODELING OF CEMENT HYDRATE: FROM ELECTRONS TO MICROTEXTURE OF C-S-H

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ABSTRACT

Calcium-Slicate-Hydrate (C-S-H) gel is the binder phase and the principal source of strength in Portland cement concretes. Despite decades of studies on C-S-H, the interplay between the structure, composition and morphology of this complex gel persists to be poorly understood. Here, we propose a bottom-up hierarchical approach developed with the focus of predicting the morphology and properties of C-S-H at the micro level based on the consequences at the subatomic levels. In particular, we show that different Ca/Si ratios present in real cement hydrate system drive the morphology and structure of C-S-H microtexture. First, using first principle calculations we develop a force field potential, CSH-FF, which is customized for the C-S-H family to reliably predict structural and mechanical properties. Next, by leveraging the CSH-FF and using a combinatorial approach, we build all possible molecular “polymorphs” of C-S-H phases for each Ca/Si ratio. By allowing for short silica chains distributed as monomers, dimers, and pentamers, these C-S-H archetypes of molecular descriptions of interacting CaO, SiO2, and H2O units provide realistic values of the Ca/Si ratios and the density computed by grand canonical Monte Carlo simulations. Second, via applying tension to the thermodynamically stable polymeric C-S-H structures, we mechanistically define particle boundaries for the hardened C-S-H phases. These particles form the microtexture of C-S-H, which is simulated by a Monte Carlo method with a coarse grain potential derived from the MD simulation. Finally, bulk modulus of a simplified model of this microtexture is predicted and compared with experiments on real C-S-H.

Keywords
C-S-H**,** first-principle calculations, combinatorial atomistic modeling, particle boundaries,