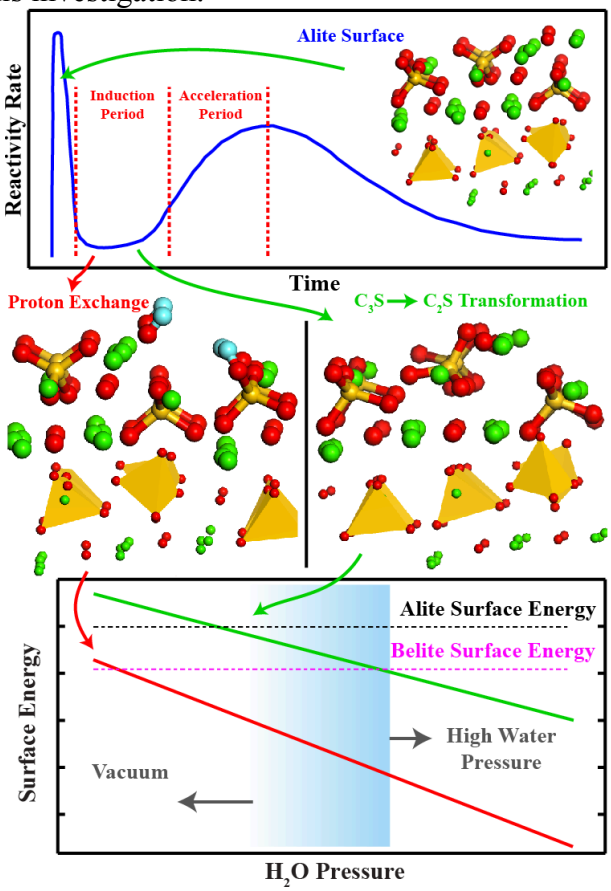
Induction Period in Alite Hydration

Problem

The hydration of cement powder involves a series of chemical stages that exhibit complex kinetics. One long-standing challenge is to understand the mechanism for the rapid decrease in the rate of dissolution of alite during early stages of hydration. This period of slow dissolution, the induction period, has great engineering significance in that during this period concrete can be transported, placed and finished before the hardening process begins. Controlling the length of the induction period is an important aspect of concrete engineering. After the induction period, the reactivity of alite increases rapidly during the first dozen or so hours. The chemical mechanisms that control the induction period are the subject of this investigation.



Transformation of an alite surface upon interaction with water. Green, yellow, red and blue spheres represent Ca, Si, O and H atoms, respectively.

Approach

First-principle fully quantum mechanical analytical techniques are applied to modeling the interface of water and alite. Combined with thermodynamic approaches, we show how pure alite (C_3S) and water interact during the very early stages of reaction. Two of the most probable mechanisms proposed in the literature for the slowing of reaction are considered: 1) that C_3S transforms into a more stable C_2S-like surface and 2) that protonation occurs, in which surface Ca atoms are exchanged with hydrogen atoms. By calculating the surface energy of the systems at varying water pressures, we predict modifications of the C_3S surface, which provides insight as to why the reactivity decreases during the induction period.

Findings

The key finding of this research is that upon increasing the water pressure, both C_2S-like and proton exchanged surfaces become more stable than the ideal C_3S surface. These two independent transformations are observed for both most and least stable surfaces of C_3S crystals. As these transformed surfaces are more stable than C_3S surfaces, the reduction in solubility rates is therefore expected. The reactivity increases back again after transformed surfaces are dissolved.

Impact

This research provides new information about the mechanisms that control the decrease in reactivity of alite during the induction period. This information can only be obtained by detailed atomic scale modeling, which provides an important piece of a complex puzzle, and brings us closer to a complete mechanistic description of the hydration process.

More

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This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association (PCA) and the Ready Mixed Concrete (RMC) Research & Education Foundation.
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