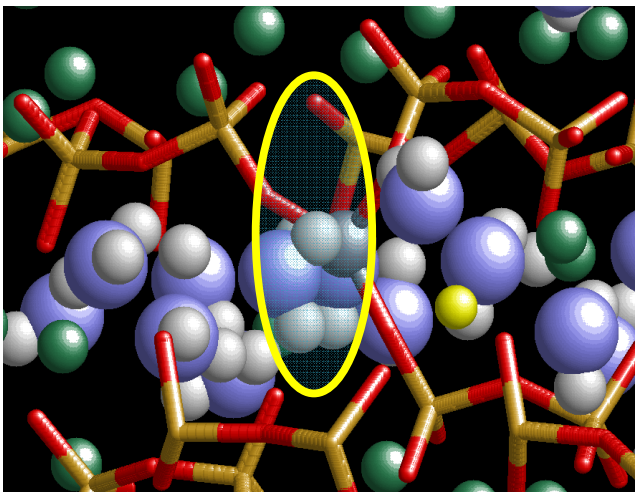
Concrete Sustainability Hub@MIT Research Profile Letter – September 2010

Fly Ash is Critical for C-A-S-H

Problem

Replacing part of the clinker with low-cost coal fly ash has recently emerged as a viable economical and ecological solution to balance material efficiency with environmental concerns. From a resource perspective, coal fly ash is still under-utilized in the industry, while it is well known to be an excellent candidate to partially replace clinker, due to the mixture of calcium and aluminum it contains. Yet, for fly ash to be safely used in concrete in larger concentrations than currently permitted, it is imperative to advance our understanding how aluminum incorporation in calcium-silicate-hydrates (C-S-H) affects the structural and chemomechanical performance of calcium-alumino-silicate-hydrates, or C-A-S-H. Theoretically, aluminum can replace either silicon or calcium atoms in the C-S-H structure. However, which form of substitution prevails in fly ash concrete continues to be an enigma that has defied many experimentally and theoretically decoding attempts.



Formation of the 3-D molecular skeleton of C-A-S-H by Ca-Al substitution. Brown-red sticks represent silica dimmers, gray and green spheres represent Al and Ca atoms, respectively. The structural water molecules are shown by blue and while spheres.

Approach

In contrast to the classical top-down empirical approaches, we have chosen a bottom-up approach that starts at the electron and atomic scale of calcium hydrates with silicon-aluminum (Si-Al) and calcium-aluminum (Ca-Al) substitution. By conducting a wide spectrum of atomistic simulation methods on thousands of aluminum containing molecular C-A-S-H structures, a consistent model emerges which congruently juxtaposes different pieces of experiments together, including Wavelength Dispersive Spectroscopy (WDS), X-Ray Diffraction (XRD) and Nuclear Magnetic Resonance (NMR) results.

Findings

The key finding of this research is that Al can substitute for Si only into silica chains of C-S-H. Because of the finite number of such chains in C-S-H, this form of substitution saturates. Beyond this saturation Al substitutes for Ca-monomers. This form of substitution creates a complex 3-D bonding scheme which enhances strength, stiffness and durability of the elementary building block of fly ash concrete.

Impact

This research highlights the beneficial role of aluminum substituting for calcium on chemical stability and performance of C-A-S-H. It suggests that a high amount of aluminum provided by a larger fly ash concentration than currently in use can enhance properties in a “bottom-up” fashion, from the molecular scale to macroscopic scale of day-to-day concrete engineering applications.

More

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