

Validating Effects of Cement Paste Composition on Mechanics

Problem

Our molecular simulations of calcium-silicate-hydrate (C-S-H), an ingredient of cement pastes fundamental to performance of concrete, predict that C-S-H of Ca/Si ~ 1 is about 25% stiffer and 60% harder than C-S-H of Ca/Si ~ 1.7 found in ordinary portland cement (OPC) pastes [1]. Here, we aim to validate this prediction experimentally.

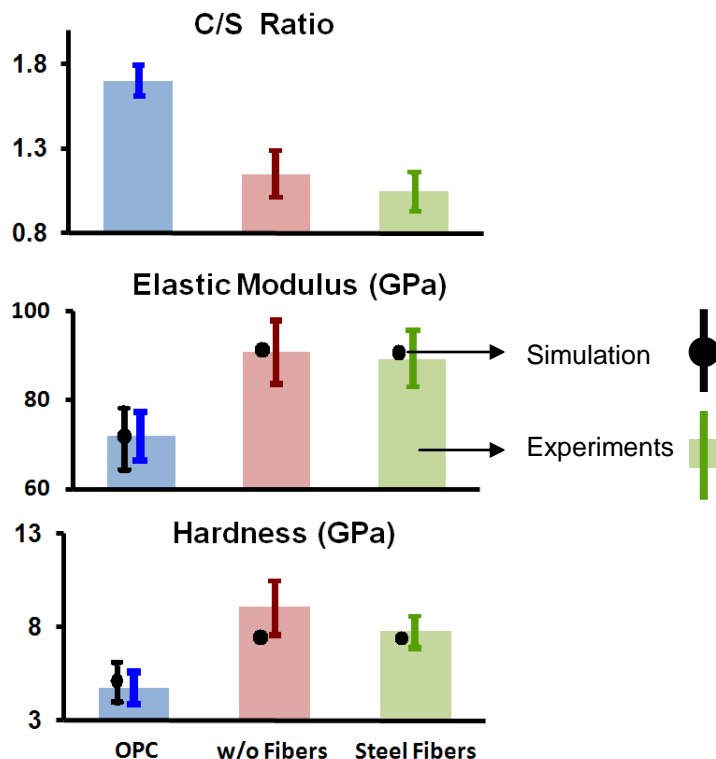
Approach

How do we experimentally realize C-S-H of Ca/Si ~ 1 ? It is known that presence of silica in cement pastes reduces the Ca/Si of C-S-H by a pozzolanic reaction. We hypothesize that silica-rich cement used in ultra high performance concrete (UHPC) could produce C-S-H of Ca/Si ~ 1 .

We utilized a commercially available UHPC to access C-S-H of Ca/Si ~ 1 and commercially available OPC paste to access C-S-H of Ca/Si ~ 1.7 . We characterize the chemical composition of C-S-H using X-ray spectroscopy. We use a combination of nanoindentation and micromechanics modeling to calculate the fundamental nanoscale stiffness and hardness of C-S-H. The details of experimental methods can be found elsewhere [2, 3].

Findings

We obtain three interesting results summarized in the figure on the right. First, we show that low C/S ratios in C-S-H are obtainable via silica-rich UHPC. Second, C-S-H of Ca/Si ~ 1 is 25% stiffer and 60% - 90% harder than C-S-H of Ca/Si ~ 1.7 typical of OPC pastes. This agrees well with predictions from our molecular simulations. Third, we find that steel fibers do not alter the fundamental mechanical properties of C-S-H significantly (within error limits).



Impact

We validate the computational prediction that Ca/Si ~ 1 creates significantly stiffer and harder C-S-H than in OPC pastes, with direct consequences for concrete performance and environmental footprint. This work shows that this Ca/Si is accessible in current, commercially available processing routes and products.

More

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[1] R. Pellenq et. al., Proc Nat Acad Sci USA 106 (2009) 16102-16107.

[2] “What’s in your concrete? (Part 1),” CSHub@MIT - Research Profile Letter Feb 2011.

[3] “What’s in your concrete? (Part 2),” CSHub@MIT - Research Profile Letter Apr 2011.



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