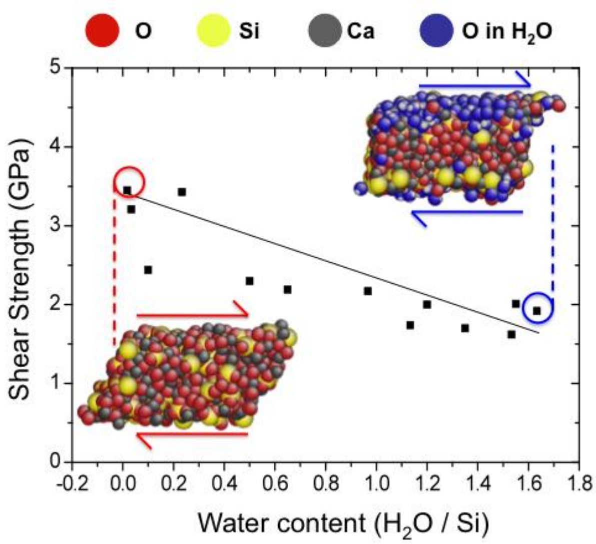
Concrete Sustainability Hub@MIT – Research Profile Letter – December 2010

C-S-H: Water, Water Everywhere

Problem

In the Rime of the Ancient Mariner, Coleridge's sailor puzzled that surrounding a ship there is "water, water everywhere, and all the boards did shrink." Indeed, the role of water in concrete properties remains a persistent challenge. The nanogranular calcium-silicate-hydrate (C-S-H) within hardened cement paste is defined by the final ratio between calcium atoms, silicon atoms, and water molecules inside each C-S-H nanoparticle. How does the mechanical stiffness and strength of a C-S-H nanoparticle change with the amount of water inside C-S-H? The answer helps to predict how concrete structures will respond to changes in humidity and temperature (e.g., due to weather or extreme environments). Such fundamental studies of water content on C-S-H properties also establish a link between the chemistry and the resulting mechanical performance of packed C-S-H nanoparticles.



As the intra-particle water content of C-S-H is changed, its shear strength changes concurrently. Atomistic simulation results indicate that a reduction of H_2O/Si from typical ratios of 1.7 to ratios of 0.2, would increases shear strength of C-S-H nanoparticles by 75%.

Approach

The number of water molecules within our molecular structure of typical C-S-H was varied via statistical mechanics. This Monte Carlo approach effectively simulates a wide range of temperatures and humidities. Mechanical properties of the resulting C-S-H phases, such as elastic moduli and shear strength, are determined via molecular simulations that deform the nanoscale phase.

Findings

This molecular model shows that the properties of calcium-silicate-hydrate depend directly on the intra-particle water content of C-S-H. In particular, the density of C-S-H nanoparticles corresponds directly to water content. Correspondingly, the stiffness and strength of the C-S-H nanoparticles vary directly with water content. C-S-H can double in strength if the water content is decreased from levels typical of hardened cement pastes.

Impact

This research highlights the importance of the water content within C-S-H on the properties of this nanoscale phase. As water content decreases, the stiffness and strength of the individual particles increases. Water content may be varied by environment, or controlled by C-S-H composition. This model can now be extended to predict how chemical composition, temperature, and humidity can affect the density and mechanical behavior of the aggregated C-S-H nanogranular phase that forms the "liquid stone" of concrete.

More

Research herein conducted by Dr. Qing (Kitty) Ji from the CSHub, in collaboration Mr. M. Youssef and Prof. B. Yildiz, and supervised by Profs. R. Pellenq and K.J. Van Vliet.

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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. The CSHub@MIT is solely responsible for content. For more information, write to CSHub@mit.edu.