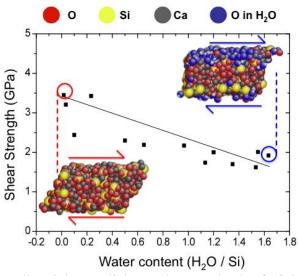
# C-S-H: Water, Water Everywhere

### **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 calcium-silicate-hydrate nanogranular within hardened cement paste is defined by the final ratio between calcium atoms, silicon atoms, molecules inside and water 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

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