Holding It Together: C-S-H Cohesion

Problem
To improve the durability of concrete under extreme conditions, it is particularly important to understand damage mechanisms within the cement paste that binds aggregates. The multiscale porosity inherent to cementitious materials implies that water may be present as liquid, solid, and/or gas depending on the thermodynamic conditions (temperature, pressure, ion concentration). It is thus appreciated that water may be both the source and the medium causing damage in cement paste. Here, computational simulations are particularly advantageous because water properties in nanoscale pores (≤1 nm) are challenging to access experimentally.

Findings
Our first key result is that cohesion within and between C-S-H grains is relatively stable down to about 20% RH, beyond which all nm-scale cement pores are filled with water. The second key result is that below 20% RH, cohesion inside a C-S-H grain is increased (grains shrink) and cohesion between C-S-H grains is decreased.

Impact
Our approach shows that cohesion within cement paste decreases with decreasing water content, specifically at RH<20% and 27°C. This loss of cohesion within the binding phase significantly affects the strength and durability of the material. These calculations help to explain reduced strength and creep resistance of concrete in very dry environments, and also provide insight toward damage mechanisms in concrete at high temperatures (e.g., fire environments) even before heat-induced polymerization of silica chains.

More
Research herein conducted by Dr. Patrick Bonnaud, postdoctoral researcher, in collaboration with Dr. Q. Ji and Prof. R. Pellenq, and supervised by Prof. K. J. Van Vliet.

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