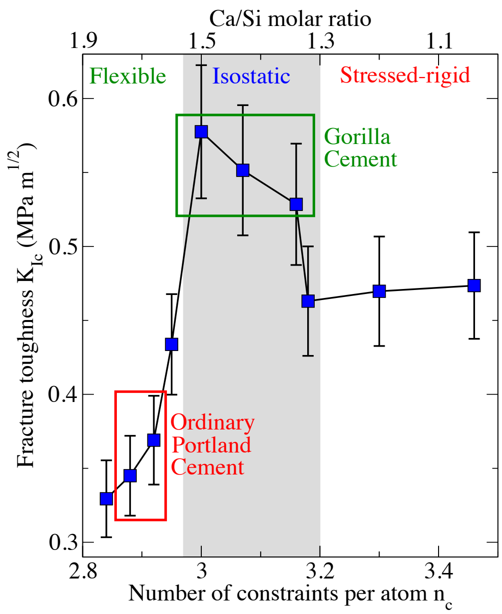
CSHub MIT CONCRETE SUSTAINABILITY HUB

Research Brief
May 2014

Gorilla cement: Tougher, yet greener

PROBLEM

Concrete is the most used construction material in the world. Thanks to its strength, durability, and low cost, it is the only material that can satisfy the growing demand for infrastructure, especially in developing countries. However, the production of cement, a key concrete ingredient, is responsible for about 5% of the human emissions of CO_2. Because of the ubiquitous presence of concrete in our society, even small decreases in CO_2 emissions due to concrete production would have a significant impact in terms of greenhouse gas emissions. To this end, one option is to improve the toughness of cement. Indeed, tougher cement would allow using less material while achieving comparable mechanical properties. Moreover, an increased resistance to fracture would improve cement's longevity, making it even more sustainable. As such, it is of primary importance to understand how composition affects the resistance to fracture of calcium-silicate-hydrates (C-S-H), the binding phase of cement, starting from the atomic scale.



Computed fracture toughness of C-S-H with respect to composition and number of constraints per atom.

APPROACH

Due to its complexity, the nanoscale structure of C-S-H is challenging to study. To understand how it affects the toughness of the material, one must filter out less significant chemical details and focus on the atomic topology that truly tunes macroscopic properties. This is precisely what rigidity theory has successfully been used to do in glass science, e.g. to design the Gorilla© glass by Corning©. It reduces complex molecular networks to simple mechanical trusses. As such, a network can be flexible, stressed-rigid, or isostatic, if, respectively, the number of chemical constraints is lower, higher, or equal to the number of degrees of freedom of the atoms. Alongside the rigidity analysis of C-S-H molecular models of varying composition (see the Research Brief of March 2013 for details), we compute by molecular dynamics simulations their respective fracture toughness.

FINDINGS

The fracture toughness of C-S-H grains is maximal for isostatic compositions, at a Ca/Si molar ratio around 1.5. This state of rigidity appears to be optimal. Indeed, stressed-rigid systems are completely locked by the high number of constraints and, consequently, tend to break in a brittle way. On the contrary, thanks to their internal degrees of freedom, flexible systems can deform and show some ductility, but their surface energy is low. Isostatic materials are able to deform and feature relatively high surface energy. Hence, we predict that decreasing the Ca/Si of C-S-H from 1.7—typical for ordinary Portland cement—to 1.5 would increase its toughness by 70%, thus allowing using less material without compromising performance. Decreasing the relative amount of calcium in cement can be achieved by replacing clinker with silica-rich byproduct materials such as fly ash. Tougher and greener, this "Gorilla cement" would help improve the sustainability of our built environment.

IMPACT

Applying glass science tools to cement provides new insights into the relationship between nanoscale composition and macroscopic properties in complex infrastructure materials. Our analysis predicts a family of compositions at which cement would show an improved toughness and, yet, a reduced environmental cost. Moreover, our methodology is generic and could be applied to optimize the composition of many materials.

This research was carried out by CSHub@MIT with sponsorship provided by the Portland Cement Association, the Ready Mixed Concrete Research & Education Foundation and Schlumberger. CSHub@MIT is solely responsible for content.
Authors: Dr. M. Bauchy, in collaboration with M. J. Abdolhosseini Qomi, Prof. F.-J. Ulm, and Dr. R. Pellenq.