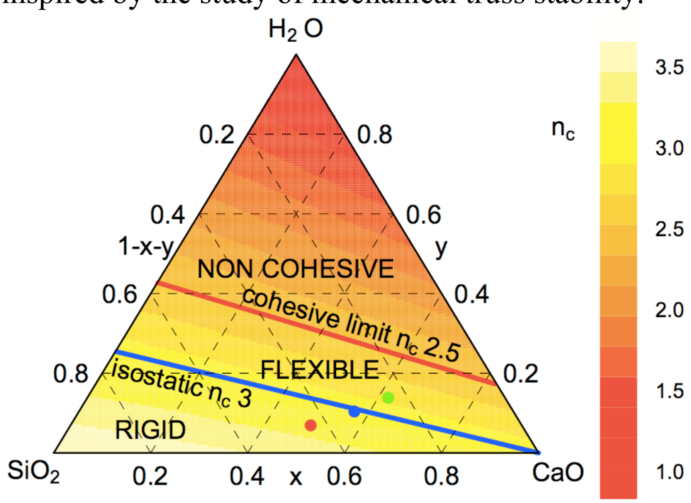
Predicting C-S-H aging

Problem

The aging of concrete is of critical importance for the industry as well as the research community. The aging process can impact performance characteristics such as creep and shrinkage and may be important in chemical reactions related to durability. In order to reduce the aging of concrete, and especially of its binding phase C-S-H, the composition of the latter might be optimized, e.g. via addition of silica fume, although a thorough understanding of the general relation between composition and aging properties is still lacking.

Approach

To study the aging of C-S-H, we used tools from glass science. Indeed, designing high-performance glass, such as Gorilla Glass® from Corning® Inc., requires a careful optimization of the composition, which is not feasible by systematic brute-force experiments or simulations of every possible mixture. This has led to the introduction of a predictive tool: the topological constraint theory, or rigidity theory. This theory relies on an enumeration of the constraints (radial two-body and angular three-body) between the atoms in the network, and is largely inspired by the study of mechanical truss stability.



Rigidity phase diagram of C-S-H with respect to its composition. The blue line indicates the durable isostatic compositions family.

When the number of constraints per atom, n_c, is less than 3 (being the number of degrees of freedom per atom), the network is said to be *flexible*. On the contrary, when $n_c > 3$, the network is *stressed-rigid* and is locked by its high connectivity. An optimal *isostatic* state is achieved when n_c=3. In the latter case, molecular networks show some remarkable properties such as a space-filling tendency, a maximum of toughness and very weak aging phenomena. Based on molecular dynamics simulations, we applied this simple but powerful theory to C-S-H samples characterized by different compositions.

Findings

We found that C-S-H shows a rigidity transition, being flexible at high Ca/Si ratio (typical of ordinary portland cement), stressed-rigid at low Ca/Si ratio and optimally isostatic around Ca/Si=1.5. The latter demonstrated a space-filling tendency at nanoscale similar to what is observed in glasses. The analysis of the constraints created by each species of atom allows one to predict the rigidity status of any composition of C-S-H as well as the existence of a family of isostatic compositions that are likely to be the most durable.

Impact

This is the first time that rigidity theory has been applied to such a complex material. Importing glass science tools to C-S-H brings new ideas to predict the effect of composition on cement aging. The use of the predicted optimal compositions of cement could lead to more durable concrete. More generally, this highlights the fact that increasing the amount of silica in cement is another means for producing green sustainable concrete.

More

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