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Cement's basic molecular structure finally decoded

Robustness comes from messiness, not a clean geometric arrangement

Denise Brehm, Civil and Environmental Engineering
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In the 2,000 or so years since the Roman Empire employed a naturally occurring form of cement to build a vast system of concrete aqueducts and other large edifices, researchers have analyzed the molecular structure of natural materials and created entirely new building materials such as steel, which has a well-documented crystalline structure at the atomic scale.

Oddly enough, the three-dimensional crystalline structure of cement hydrate - the paste that forms and quickly hardens when cement powder is mixed with water - has eluded scientific attempts at decoding, despite the fact that concrete is the most prevalent man-made material on earth and the focus of a multibillion-dollar industry that is under pressure to clean up its act. The manufacture of cement is responsible for about 5 percent of all carbon dioxide emissions worldwide, and new emission standards proposed by the U.S. Environmental Protection Agency could push the cement industry to the developing world.

"Cement is so widely used as a building material that nobody is going to replace it anytime soon. But it has a carbon dioxide problem, so a basic understanding of this material could be very timely," said MIT Professor Sidney Yip, co-author of a paper published online in the Proceedings of the National Academy of Sciences (PNAS) during the week of Sept. 7 that announces the decoding of the three-dimensional structure of the basic unit of cement hydrate by a group of MIT researchers who have adopted the team name of Liquid Stone.

"We believe this work is a first step toward a consistent model of the molecular structure of cement hydrate, and we hope the scientific community will work with it," said Yip, who is in MIT's Department of Nuclear Science and Engineering (NSE). "In every field there are breakthroughs that help the research frontier moving forward. One example is Watson and Crick's discovery of the basic structure of DNA. That structural model put biology on very sound footing."

Scientists have long believed that at the atomic level, cement hydrate (or calcium-silica-hydrate) closely resembles the rare mineral tobermorite, which has an ordered geometry consisting of layers of infinitely long chains of three-armed silica molecules (called silica tetrahedra) interspersed with neat layers of calcium oxide.

But the MIT team found that the calcium-silica-hydrate in cement isn't really a crystal. It's a hybrid that shares some characteristics with crystalline structures and some with the amorphous structure of frozen liquids, such as glass or ice.

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At the atomic scale, tobermorite and other minerals resemble the regular, layered geometric patterns of kilim rugs, with horizontal layers of triangles interspersed with layers of colored stripes. But a two-dimensional look at a unit of cement hydrate would show layers of triangles (the silica tetrahedra) with every second, fifth or eighth triangle turned up or down along the horizontal axis, reaching into the layer of calcium oxide above or below.

And it is in these messy areas - where breaks in the silica tetrahedra create small voids in the corresponding layers of calcium oxide - that water molecules attach, giving cement its robust quality. Those erstwhile "flaws" in the otherwise regular geometric structure provide some give to the building material at the atomic scale that transfers up to the macro scale. When under stress, the cement hydrate has the flexibility to stretch or compress just a little, rather than snapping.

"We've known for several years that at the nano scale, cement hydrates pack together tightly like oranges in a grocer's pyramid. Now, we've finally been able to look inside the orange to find its fundamental signature. I call it the DNA of concrete," said Franz-Josef Ulm, the Macomber Professor in the Department of Civil and Environmental Engineering (CEE), a co-author of the paper. "Whereas water weakens a material like tobermorite or jennite, it strengthens the cement hydrate. The 'disorder' or complexity of its chemistry creates a heterogenic, robust structure.

"Now that we have a validated molecular model, we can manipulate the chemical structure to design concrete for strength and environmental qualities, such as the ability to withstand higher pressure or temperature," said Ulm.

CEE Visiting Professor Roland Pellenq, director of research at the Interdisciplinary Center of Nanosciences at Marseille, which is part of the French National Center of Scientific Research and Marseille University, pinned down the exact chemical shape and structure of C-S-H using atomistic modeling on 260 co-processors and a statistical method called the grand canonical Monte Carlo simulation.

Like its name, the simulation requires a bit of gambling to find the answer. Pellenq first removed all water molecules from the basic unit of tobermorite, watched the geometry collapse, then returned the water molecules singly, then doubly and so on, removing them each time to allow the geometry to reshape as it would naturally. After he added the 104th water molecule, the correct atomic weight of C-S-H was reached, and Pellenq knew he had an accurate model for the geometric structure of the basic unit of cement hydrate.

The team then used that atomistic model to perform six tests that validated its accuracy.

"This gives us a starting point for experiments to improve the mechanical properties and durability of concrete. For instance, we can now start replacing silica in our model with other materials," said Pellenq.

Other team members are graduate student Rouzbeh Shahsavari of CEE and Markus Buehler, MIT's Esther and Harold E. Edgerton Career Development Associate Professor of Civil and Environmental Engineering; Krystyn Van Vliet, MIT's Thomas Lord Associate Professor of Materials Science and Engineering; and NSE postdoctoral associate Akihiro Kushima.

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