In a bid to develop a deeper understanding of concrete – the world's most widely used building material, Rice University scientists have now detailed previously unexplored aspects which affect the amount of energy required to make it, as well as the greenhouse gases that are subsequently released.

Rouzbeh Shahsavari, the Rice Laboratory of Materials scientist, developed techniques to analyze and see dislocations in dicalcium silicates (aka belite), of which are a component of Portland cement. He further detailed how much each of the five distinct types of belites contributes to concrete's ease of manufacture and ultimate strength.

So why has it taken this long to explore belites and their relation to varying concrete characteristics and manufacturing factors? As stated by Shahsavari, "Though belite is crystalline in nature, the crystals are so small and the material so amorphous that nobody has looked at them with the kind of analytical eye they deserve." Shahsavari continues to explain that by fine-tuning belite for use in cement that holds concrete together can ultimately help save energy which in turn would lead to reductions in CO2 emissions.

"Putting an atomistic lens on the role of defects on the mechanics and water reactivity of belite crystals can provide new insights on how to modulate the grinding energy of cement clinkers and strength development of concrete," he said. "Both of these factors can significantly contribute to energy saving and reduced environmental footprints due to the use and manufacture of concrete."

In comparison to tricalcium silicate – a dominant ingredient in cement, belite has the advantage of being produced at a much lower temperature (at least 100 degress Celsius lower). However, one issue that arises is with respect to the fact that belite is harder to grind and tends to react more slowly with water. This in turn leads to delayed strength development in cement paste. Shahsavari stated that although these issues have essentially curbed the wide-spread use of belite-based cement in concrete, his lab has adapted an approach that could bring change.

Belite crystals of calcium, silicon and oxygen mainly take one of two different forms, either monoclinic or orthorhombic, each of which behaves differently at the atomic level. These were then subdivided into into five distinct polymorphic crystals. Then, through computer simulations and high-resolution electron microscopy, it was determined that one of the monoclinic forms, the beta-C2S, is the most brittle and possibly the best-suited for cements requiring low-energy manufacture.

Shahsavari said the research provides new insight about the bottom-up engineering of materials that have the properties of cement. "The physical understanding gained by our high-resolution electron microscopy images, the first of their kind for cement, combined with our atomistic-level computations, can put cement-based materials on equal footing with metallic systems and semiconductors in the emerging application of 'defect-engineering' to boost performance in manufacturability and functionality," he said. "We expect this will lead to energy savings and environmental benefits."

Source: https://www.eurekalert.org/pub_releases/2016-10/ru-rul100316.php