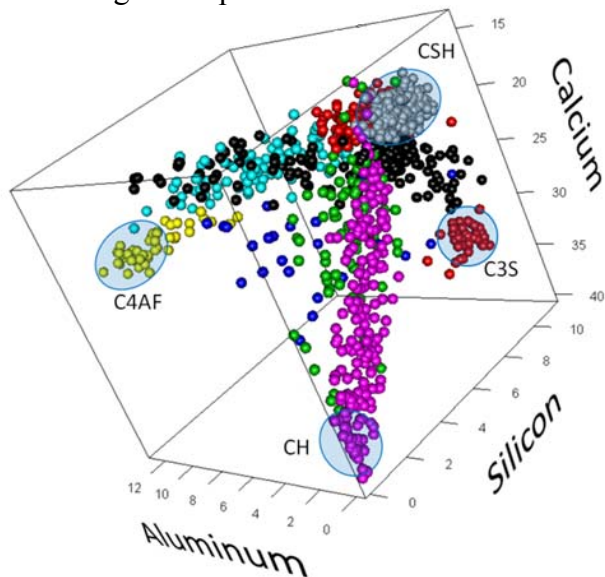


What's in Your Concrete? (Part 1)

Problem

Concrete is defined by its properties in the hardened state. However, these are known to depend strongly on the chemical make-up created by the tens of chemical hydration reactions that take place when cement clinker phases react to form this cohesive liquid stone. The difficulty in reliable assessment of this chemical signature stems from the many possible combinations and spatial distributions of different elements (Si, Ca, Al, Fe, Mg, S, Na, etc.) that make up the multiple phases within the cement paste. These phases include calcium-silicate-hydrates (C-S-H), portlandite (CH), aluminates, and unhydrated clinker. Additions of slag, fly ash, silica fume, limestone, and other chemically complex phases significantly add to this challenge. To relate the *in situ* chemistry to the mechanical performance of the binding phase of concrete, new experimental and analytical tools are required. Such capabilities will afford control and validation of new models and prototype cements to attain industry-wide goals including lowering the greenhouse gas components of concrete.



In situ assessment of cement chemistry by statistical cluster analysis of wavelength dispersive spectra for a specific Portland cement (OPC). Colors represent different phases in hardened cement paste as identified by this analysis. Units in atomic percent (number of atoms/total number; except H).

Approach

We employ a statistical clustering algorithm to translate experimental measurements into a chemical signature of each cement paste. These experiments employ an electron microprobe to collect X-ray wavelength dispersive spectra (WDS) at many points on the sample surface. Each point in this array is a three-dimensional pixel of μm -scale volume, or a voxel, and a massive array is acquired (e.g., >1000 voxels over $\sim 1\text{mm}^2$). The results are then analyzed via a clustering algorithm. This approach employs expectation maximization to assign each voxel to the most probable cluster. Each cluster is representative of a chemically distinct phase within the hardened cement or concrete. The number of unique clusters is identified via Bayesian statistics, and the cluster volume fraction is determined from the number of voxels comprising that phase.

Findings

This cluster analysis quantifies chemical composition and volume fraction of cement paste phases, as a function of mixture design and environmental exposure.



Impact

This research combines *in situ* X-ray spectra and multivariate statistics to characterize quantitatively the chemical signature and volume fraction of phases in hardened cement paste. The comparable size of voxels in this chemical analysis and our nanomechanical characterization now provides both an indispensable tool to link cement chemistry to nanoscale mechanical properties and engineering performance of cement and concrete.

More

Research herein conducted by Muhannad Abuhaikal, graduate student in the CSHub, in collaboration with Drs. K. Stewart and J.A. Ortega, and supervised by Profs. K.J. Van Vliet and F-J. Ulm.

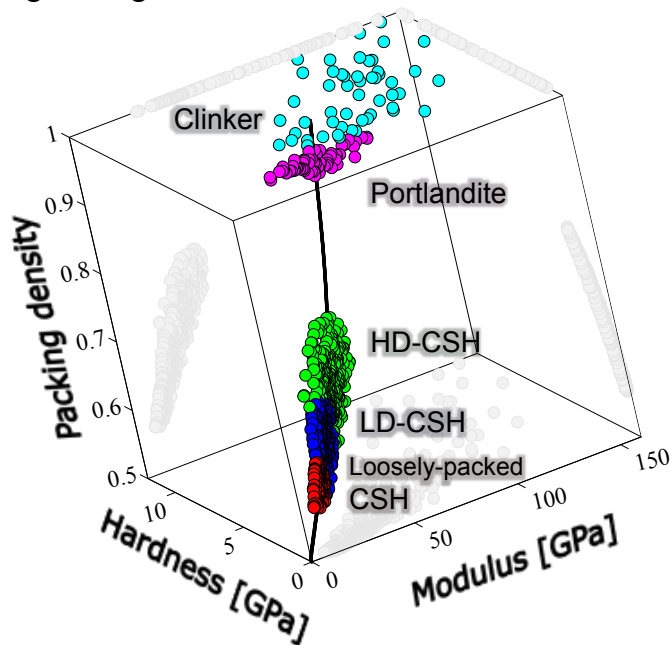


This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association (PCA) and the Ready Mixed Concrete (RMC) Research & Education Foundation. The CSHub@MIT is solely responsible for content. For more information, write to CSHub@mit.edu.

What's in Your Concrete? (Part 2)

Problem

In the transition from liquid to stone, the complex chemical hydration reactions in concrete define a highly heterogeneous composite. The multiscale nature of the hardened material, with solids and pore spaces occurring across the nano-to-macro length spectrum, poses a challenge when linking the contributions of different constituents to the overall mechanical performance. Particularly difficult is pinning down the mechanical properties of the calcium silicate hydrate (C-S-H) phase. A dedicated experimental arrangement with high resolution is required to assess in situ the engineering properties of the components in the cement binder. The direct probing of cement at the scale of C-S-H, where mechanics meets chemistry, will allow decoding the effects of mix design and environmental exposure on material performance, and thus help the nano-engineering of future blends.



In situ assessment of cement mechanics by statistical cluster analysis of nanoindentation properties for a portland cement. Colors represent different mechanical phases in the hardened cement paste, with low (LD) and high-density (HD) CSH being dominant by volume fraction. Hardness and modulus measurements relate to strength and elastic properties, respectively.

Approach

We employ a statistical clustering algorithm and micromechanics models to translate experimental measurements into a mechanical assessment of each cement paste. The experiments involve instrumented indentations at many locations on the sample surface. Stiffness and hardness properties are inferred from the load-deformation response measured in each experiment. Although probing the surface, an indentation probe effectively senses a material volume, or voxel. A massive array of indentations are conducted and analyzed via clustering statistics, which assign each voxel to a most probable cluster representative of a mechanically distinct phase within the hardened cement paste.

Findings

The dominating phases of C-S-H reveal a unique mechanical signature expressed in two material packings, a low density (LD) and a high density (HD) C-S-H phase. A small volume fraction of loosely-packed C-S-H can be found in regions affected by capillary pores. LD C-S-H dominates in high w/c ratio materials, while HD C-S-H prevails in low w/c materials; which shows that the packing of C-S-H translates directly into macroscopic strength and durability performance.



Impact

This research combines nanoindentation and multivariate statistics to characterize quantitatively the mechanical response and volume fractions of phases in hardened cement paste. The comparable size of voxels in this mechanical analysis and our chemical characterization provides a formidable tool to relate mechanical performance to cement and concrete chemistry.

More

Research conducted by Muhannad Abuhaikal, graduate student in the CSHub, in collaboration with Dr. J.A. Ortega, and supervised by Profs. K.J. Van Vliet and F-J. Ulm.



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