Cement: a Multi-scale Porous Material Under the Nanoscope

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Setting up the stage, one can list important engineering problems such as hydrogen storage for transportation applications, electric energy storage in batteries, CO_2 sequestration in used coal mines, earthquake mechanisms, durability of nuclear fuels, stability of soils and sediment and cement and concrete cohesive properties in the context of sustainability. With the exception of health, these are basically the challenging engineering problems of the coming century that address energy, environment and natural hazards.

Behind all those problems are complex multi-scale porous materials that have a confined fluid in their pore void: water in the case cement and clays, an electrolyte in the case of batteries and super-capacitors, weakly interacting molecular fluids in the case of hydrogen storage devices (H_2), gas-shale (CH_4) and nuclear fuel bars (Xe).

So what do we mean by “under the nanoscope” ? The nanoscope does not exist as a single experimental technique able of assessing the 3D texture of complex multiscale material. Obviously techniques such as TEM are part of the answer but are not the “nanoscope” in itself. In our idea, the “nanoscope” is more than a technique producing images. It is rather a concept that links a suite of modeling techniques coupled with experiments (electron and X-rays microscopies, tomography, nanoindentation, nanoscratching...). If properly defined, the nanoscope should allow accessing material texture, chemistry, mechanical behavior, and adsorption/condensation behavior at all scales starting from the nanoscale upwards in a bottom-up fashion. The toolbox of the simulation aspect of the "nanoscope" is akin to a statistical physics description of material texture and properties including the thermodynamics and dynamics of the fluids confined to their pore voids as a means to linking atomic scale properties to macroscopic properties and behaviors. The “Art of simulation” includes the description of realistic multiscale porous materials samples at atomic scales, the set up and the validity checking of transferable interatomic/intermolecular/interparticle potentials, Grand canonical Monte Carlo and Molecular Dynamics simulation techniques with the goal of probing mechanical (elasticity, strength, fracture energy), adsorption (fluid condensation/evaporation/docking) and transport properties (permeablility, etc...).

By contrast, the engineering toolbox consists in continuum or discrete models, which are either based on or focused on mean field theories like continuum theories that usually neglect thermal fluctuations and are assumed to a obey equilibrium thermodynamics at least in a macroscopic formulation based on adjusting variables on limiting simpler cases. Both routes aim at predicting material properties. Ideally, the “dream” would be to have a unified engineering/ physical approach consistent from the scale of atoms to the scale of continuum theories, to tackle the challenging problems evoked here above. In this talk, I will specifically address the case of cement hydrate (CSH), the glue that gives concrete its remarkable mechanics properties by putting "CSH under the nanoscope".

Figure: Cement from atoms to applications [Pellenq et al, PNAS 2009]