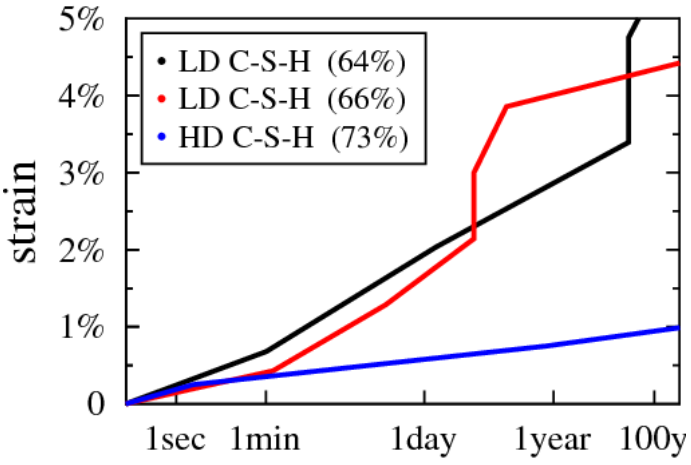
Nano–Engineering Creep

Problem

Creep is the accumulation of irreversible deformation under constant load over time. Understanding and controlling the microscopic mechanisms of deformation that underlie creep is a prerequisite to the development of new, even more durable concretes. Traditional models are based on phenomenological rules that assume certain a priori mechanisms. However, the tremendous number of possible mix-designs demands tools to predict and engineer the mechanisms of creep deformation. Direct simulations are suitable for such detailed studies, but are limited to time scales of few nanoseconds. Creep instead spans a huge range of time scales, from the nanoseconds of molecular processes to the years of macroscopic deformations. Hence, there is a need for new modeling techniques that can capture the multi-scale, long-term kinetics of cement paste deformation.



Creep curves for low-density (LD) C-S-H gels (solid fractions 64% and 66%) and high-density (HD) C-S-H gels (solid fraction 73%). The applied shear stress is 100 MPa for the LD C-S-H systems, and 280 MPa for the HD one (70% of the failure stress in both cases). The horizontal axis of time is in logarithmic scale. The linear trends of the strain in this scale indicate logarithmic creep. Note that the HD gel creeps much less than the LD ones.

Approach

We consider model structures of C-S-H gels with different solid fractions, at the scale of ~100 nm. The structures are composed of colloidal nanoparticles that interact via cohesive forces derived from the smaller molecular scale. The model structures are probed via simulations of quasi-static shear tests, from which we compute the activation energy for the accumulation of irreversible strain. The Transition State Theory then allows converting the activation energies to time required for irreversible deformations.

Findings

We capture the logarithmic creep regime observed in experiments at microscopic as well as macroscopic scales. The logarithmic regime covers a wide range of time scales. In agreement with nanoindentation experiments, the results of our model indicate that the high-density C-S-H has a smaller tendency to creep compared to the low-density C-S-H. We obtain creep moduli in the range of tens to hundreds of GPa, which also agrees well with nanoindentation experiments. Preliminary results at the molecular scale seem to capture the important effect of water content on the creep of the C-S-H, namely that a low water content slows down the creep.

Impact

We have shown that the multi-scale logarithmic creep can be predicted from direct simulations at fundamental scales. This lays the groundwork for an unprecedented understanding of the mechanisms that govern the creep of cement pastes. Controlling these mechanisms is one key advance toward new design paradigms for more durable concretes.

More

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