

Resilience at high temperatures

PROBLEM

Understanding of cement damage processes is key to designing new approaches that increase durability of cement and concrete. Resilience, defined here as resistance to degradation of mechanical properties under extreme environments typical of building fires, is of particular interest. Under such conditions, chemical and physical transformations in cement paste occur, with underlying mechanisms remaining poorly understood. Further, it is plausible that the high temperatures can affect hydrated cement phase water contents at the nanoscale sufficiently to alter the microstructure and thus reduce macroscale damage tolerance or failure strength. Here we employ computational modeling and simulation to quantify the effects of elevated temperature on the physical and mechanical properties of the primary binding phase within concrete.

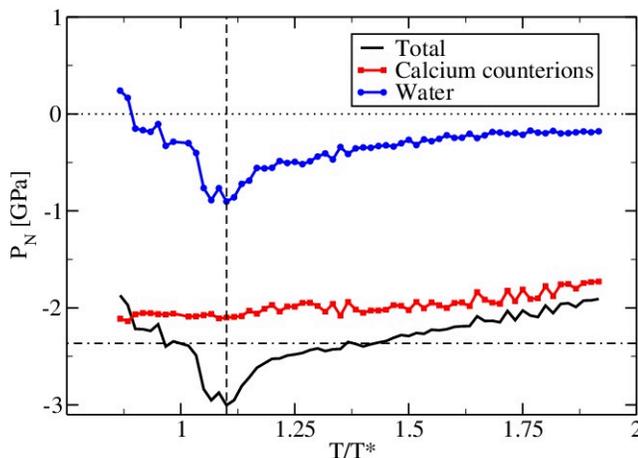


Fig. 1: Pressure (P_N) applied by the fluid confined between particles in the direction normal to the particle surface as a function of the relative temperature T/T^* . The total fluid pressure (black) can be considered the sum of that due to the water molecules (blue) and the calcium ions (red). Negative pressure indicates particle cohesion, which is reduced for $T/T^* > 1.1$.

APPROACH

Our study focuses on calcium-silicate-hydrate (C-S-H), the chief binding phase in hydrated cement and concrete. We employ Grand Canonical Monte Carlo techniques to consider how the water content between C-S-H nanoparticles changes as a function of the relative temperature T/T^* . Here, T^* is the transition temperature at which the bulk liquid and gas are in equilibrium for a given pressure (e.g., $T^* = 100^\circ\text{C}$ for bulk water at ambient pressure). Cohesion between C-S-H particles is related to the strength of the binding phase. To relate the effect of the water content on cohesion, we computed virial pressures due to the pore fluid (water and calcium ions) perpendicular to the particle surface. Negative pressure expresses a cohesive or attractive behavior, and positive pressure expresses a disjoining or repulsive behavior. We considered a situation for which the fluid is confined between two C-S-H particles of a Ca/Si ratio of 1.65 and separated by a distance of 1 nm. This reflects the estimated composition and interparticle spacing of typical cement pastes.

FINDINGS

Water content within particles decreased with increasing relative temperature up to $T/T^* = 2$, and C-S-H particles densified with attendant increases in heat capacity, stiffness, and hardness. Interparticle cohesion (Fig.1) increased up to a relative temperature of $T/T^* = 1.1$ and then decreased at higher relative temperatures. This suggests a rationale for the decreased mechanical performance of cement paste and concrete at high relative temperatures, and supports previous claims of peak hardness in C-S-H at an intermediate T/T^* between 1 and 2.6. While calcium ions modulate cohesion within cement paste, these atomistic studies underscore the important role of confined water in modulating the cohesion and, thus, the structure and properties of cement paste under extreme thermal environments.

IMPACT

These calculations on C-S-H resilience provide insight toward damage mechanisms in concrete at high temperatures (e.g., fire environments) that precede polymerization of silica chains.

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