

When Concrete Takes (part of) the Heat

Problem

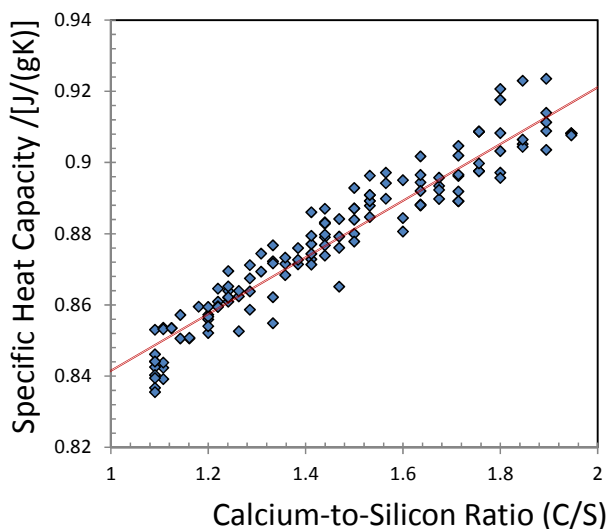
According to the U.S. Energy Information Administration, buildings consume roughly 40% of total energy use in the United States, and approximately 44% of this energy is utilized for heating and cooling. From a materials perspective, one key parameter that affects the energy efficiency of buildings is the thermal mass, which describes how the mass of the building provides "inertia" against outside temperature fluctuations (e.g. day and night). The thermal mass absorbs thermal energy when the surroundings are higher in temperature than the mass, and gives thermal energy back when the surroundings are cooler. From a physics point of view, thermal mass is equivalent to thermal capacitance or heat capacity, that is, the ability of a body to store thermal energy. While it is well known that the specific heat capacity of a material is a function of its structure, the link for cement paste has not been studied. The molecular models developed at MIT, however, lend themselves to just this type of investigation. Thus, the question this research addresses is what, if any, is the relationship between structure and chemistry of calcium silicate hydrates (C-S-H), the molecular glue of concrete, and specific heat capacity.

Approach

The calculation of heat capacity of C-S-H is performed via an original step-by-step atomistic simulation approach recently developed at MIT. A large variety of C-S-H structures of different calcium-to-silicon ratios (C/S) is constructed from which specific heat capacity is computed: First, a Grand Canonical Monte-Carlo simulation of water absorption introduces water into the nanopores of imperfect C-S-H structures. Then, a lattice dynamics Gibbs free energy minimization is performed to find the atomic structure at thermodynamic equilibrium. Finally, a series of phonon calculations provide a direct means of determining the specific heat capacity.

Findings

The general trend is that the specific heat capacity of C-S-H, at room temperature, increases with C/S. This increase is a combined result of the glassy structure and (structural) water content of C-S-H. Increasing the C/S ratio results in C-S-H structures that have weaker bonds (CaO vs. SiO), which can host more water molecules. Weaker bonds favor a higher heat capacity, as does the concurrent increase in confined water content.



Specific heat capacity vs. calcium-to-silicon ratio (C/S) for different molecular C-S-H structures.

Impact

This research highlights the impact of chemical modifications, namely the calcium-to-silicon ratio, on specific heat capacity of C-S-H. It also highlights the power of the bottom-up approach being developed at MIT. Specifically, the derived functional relations between thermal properties and molecular structures provide a molecular baseline for nanoengineering the thermal performance of cement-based materials that will eventually contribute to increasing the energy efficiency of buildings.

More

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