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Stress relaxation properties of calcium silicate hydrate: a molecular dynamics study

Key words: Calcium-silicate-hydrate; Stress relaxation; Ca/Si ratio; Temperature; Water content; Atomic simulation

Corresponding author: Shengwen TANG

Email: tangsw@whu.edu.cn

ORCID: https://orcid.org/0000-0002-4883-3103

Motivition

1. The time-dependent viscoelastic response of cement-based materials to applied deformation is far from fully understood at the atomic level.

2. Calcium silicate hydrate (C-S-H), the main hydration product of Portland cement, is responsible for the viscoelastic mechanism of cement-based materials.

3. The effects of various factors on the stress relaxation properties of C-S-H were systematically investigated by molecular dynamics simulation to shed light on the stress relaxation properties of C-S-H from a microscopic perspective, bridging the gap between the microscopic phenomena and the underlying atomic-level mechanisms.

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Method

■ Evolution of stress

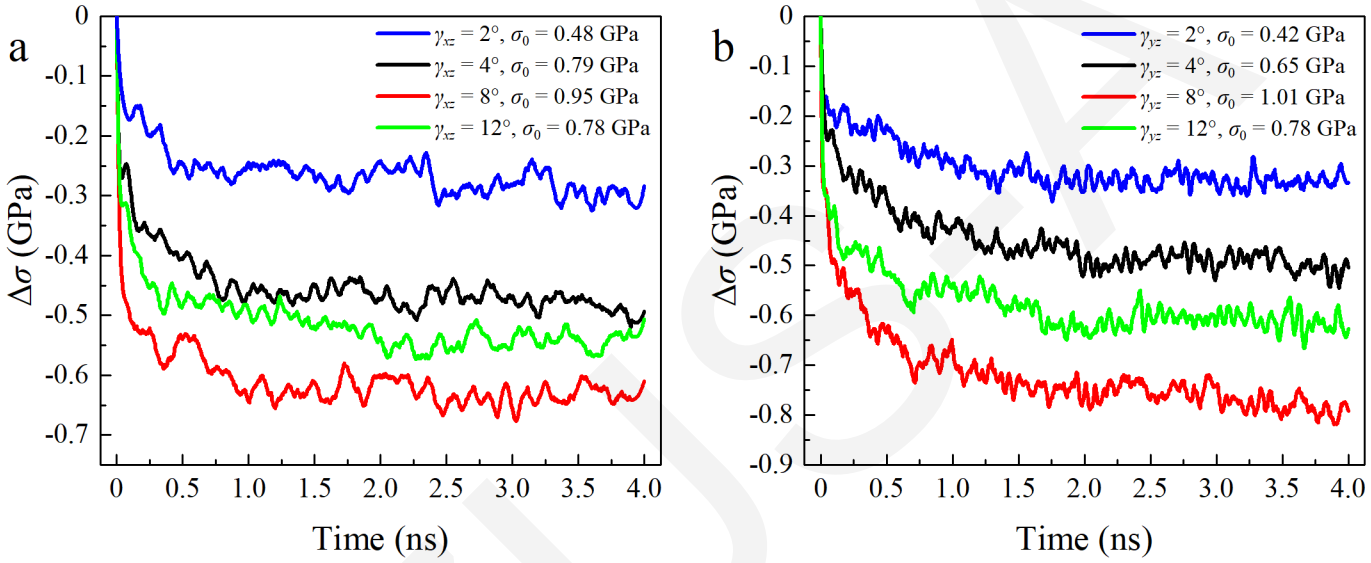

Fig. 4 The change in stress of C-S-H subjected to different shear deformations at T = 298 K: (a) evolution of $\Delta\sigma$ under γ_{xz}; (b) evolution of $\Delta\sigma$ under γ_{yz}

- The stress evolution of the entire C-S-H system takes on a typical L-shape during the stress relaxation process.
- once the initial shear deformation exceeds the elastoplastic range, some micro cracks are probably generated within C-S-H systems, resulting in a rela-tively small $\Delta\sigma$ during the stress relaxation process

Method

■ Time correction function

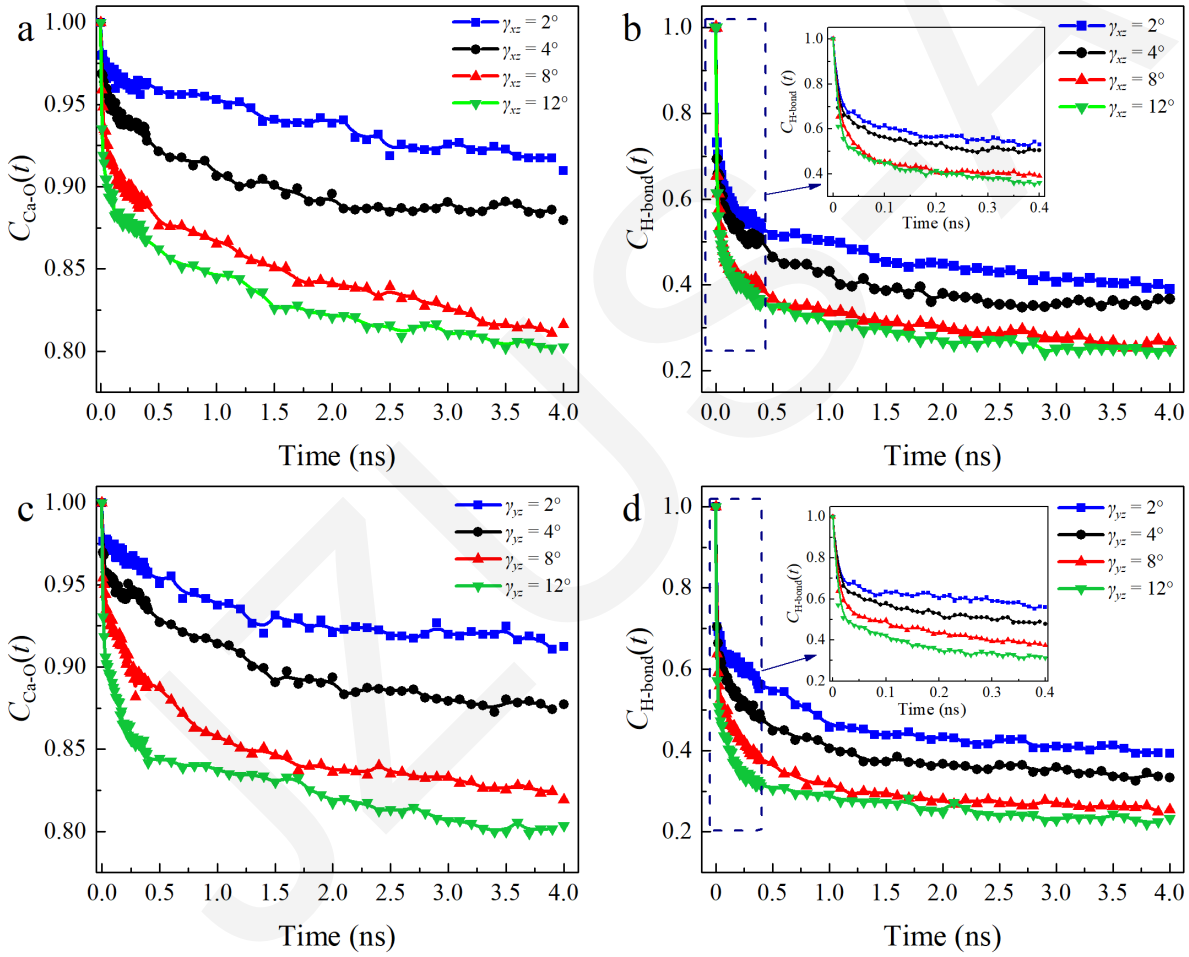

Fig. 7 *C(t)* of the interlayer Ca-O bonds and H-bonds under different shear states considered here: (a) *C(t)* of interlayer Ca-O bonds under γ_{xz}; (b) *C(t)* of H-bonds under γ_{xz}; (c) *C(t)* of interlayer Ca-O bonds under γ_{yz}; (d) *C(t)* of H-bonds under γ_{yz}.

Method

■ Mean square displacement

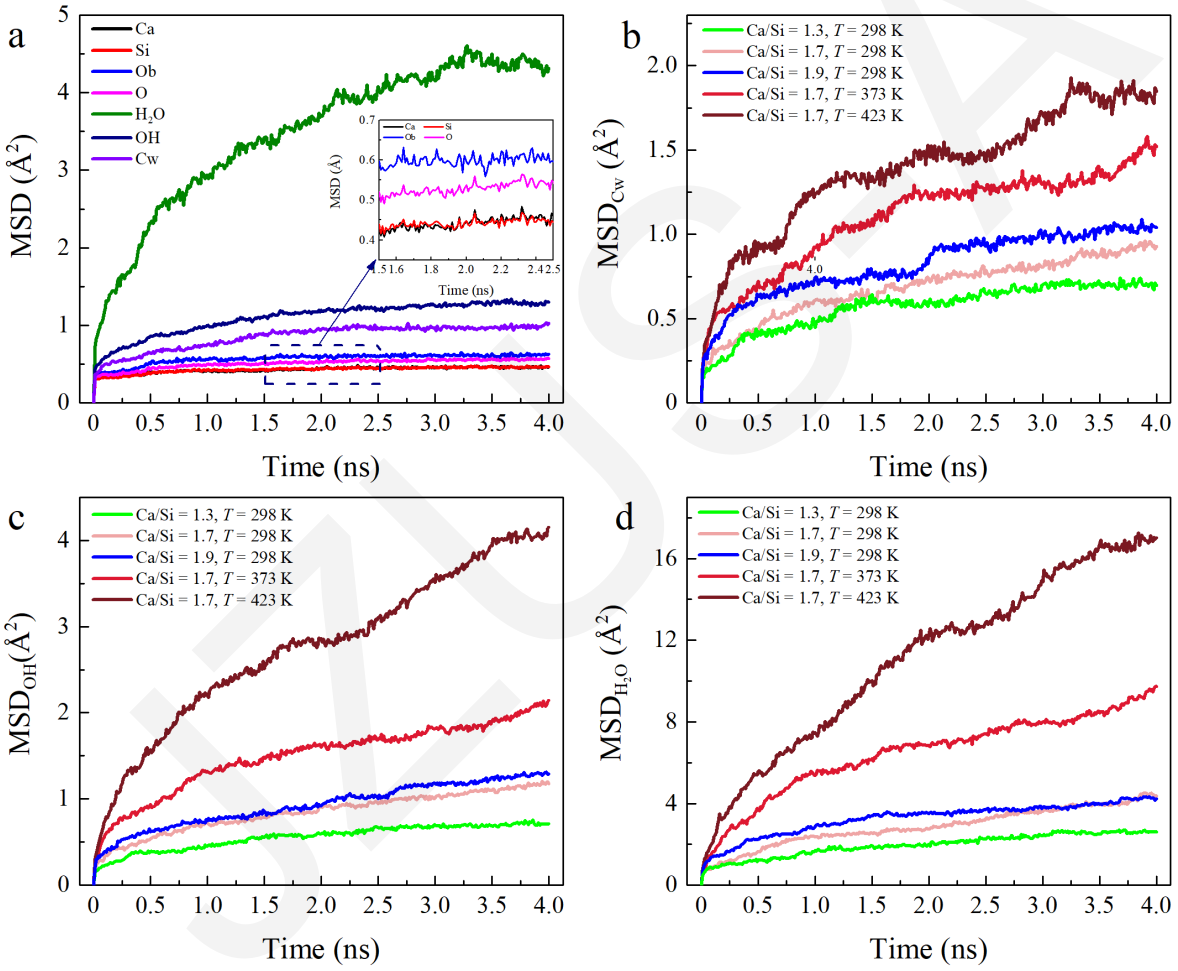

Fig. 11 MSD of constituent parts in the C-S-H system under γ_{xz} = 4° : (a) MSD of each atom/molecule/group in C-S-H at T = 298 K; (b) MSD of interlayer calcium; (c) MSD of hydroxyl group; (d) MSD of water molecule.

Method

■ Nonaffine squared displacement

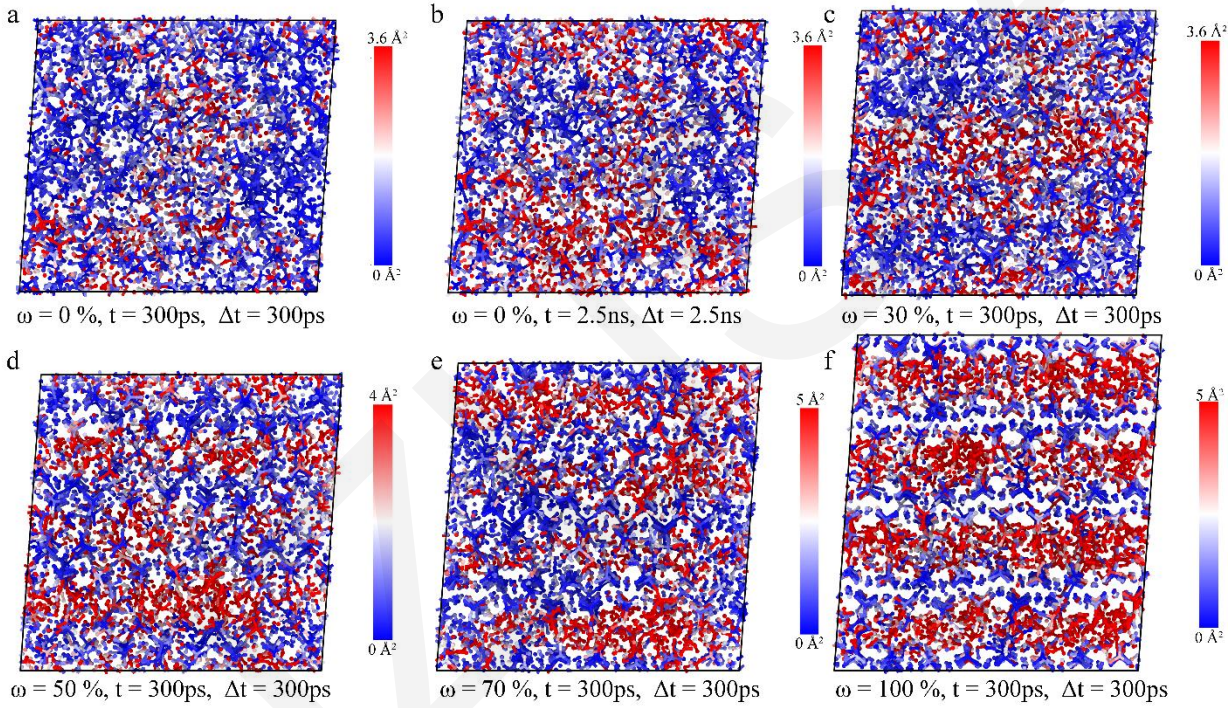

Fig. 15 Intensity plots of nonaffine squared displacement of C-S-H system with different water contents (r_{cut} = 3 Å).

Conclusions

- The stress relaxation response of C-S-H occurs regardless of whether it is under initial shear, tensile, or compressive deformation, and shows a heterogeneous characteristic.
- A large Ca/Si ratio or high temperature leads to low viscosity in the interlayer region and low cohesion between the calcium-silicate layer and the interlayer region, resulting in high atomic dynamics, especially for water molecules, hydroxyl groups, and interlayer calcium atoms.
- Water molecules play a critical role in the morphology and interlayer hydrogen bonding network of C-S-H, which in turn leads to C-S-H exhibiting different stress relaxation properties at different water contents.