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Cement modeled as poly-dispersed assemblage of disk-like building blocks

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ABSTRACT

Cement cohesion is closely related to calcium-silicate-hydrate gel, the major hydration product in cement, which has an elusive microstructure. It is widely accepted that cement is a poly-dispersed colloidal system encompassing disk-like building blocks. Here, we propose a coarse-grained model representing cement as an assemblage of disk-like building blocks. The interaction between pairwise building blocks is governed by a modified Gay-Berne potential. The coarse-grained model shows that relatively large beads could serve as the major load-bearing constituent in cement.

1. INTRODUCTION

Concrete is the most widely used construction material in the world. Mechanical performance of concrete highly depends on cement, the cohesive phase that binds various grains and clinkers together. Cement gains its cohesive strength from hydration and hardening, which encompass growth of hydration products from nanoscale to micron scale. The major hydration product in cement is the calcium-silicate-hydrate (C-S-H), which essentially determines the mechanical behavior of cement paste. The cement hydration mechanism, the development of C-S-H microstructure and the mechanical properties of cement are closely related with each other (Jennings 2000). Knowledge of such relationship provides a theoretical basis for designing and producing more sustainable concrete. At the length scale of several hundred nanometers, experimental studies have revealed that C-S-H is a heterogeneous material composed of variously sized building blocks (Jennings 2000; Chiang, Fratini et al. 2012). These building blocks are disk-like objects with approximately 1-nm thickness and 5 to 10-nm diameter. Following this concept, we model the C-S-H system as an assemblage of disk-like units and aim to study how the particle size distribution affects the mechanical properties of cement paste. We simulate C-S-H samples with controlled particle size distributions. The dependence of mechanical property on the particle size distribution is presented.

2. PROPOSED COARSE-GRAINED MODEL

2.1. Use of GB potential for describing interaction between pairwise disks

We adopt the Gay-Berne (GB) potential (Gay and Berne 1981) to simulate disk-like plates. The GB potential is initially developed for describing interactions between ellipsoidal beads and is used here to govern the pairwise interaction between disk-like C-S-H building blocks. Considering an ellipsoid with three radii a, b, and c, when c is much smaller than a, b, the ellipsoid becomes akin to a disk-like plate. Thereby the GB potential can be used for describing interactions between disk-like objects. When defining the interaction parameters of GB potential, we assume that the adhesion energy per unit area is constant for all particles. The normalized adhesion energy is 450 mJ/m^2, which is obtained from atomic simulations.

2.2. Construction of poly-dispersed systems

We model three 2-d systems. Initially, the CG model is set up by aligning 900 (30×30×1) beads in a 480×480×1 nm^3 simulation box with randomly assigned bead orientation. Sample 1 has a uniform size distribution, sample 2 contains more small beads and sample 3 contains more large beads. With time step set to 1 fs, the system is equilibrated for 10 ns in NPT ensemble with temperature and pressure controlled at 300 K and 1 atm respectively. After equilibration, we deform the simulation box (every 100 ps the system deforms 0.01%, the strain eventually reaches to 0.1%) and measure the stress of the modelled C-S-H in response to the deformation.

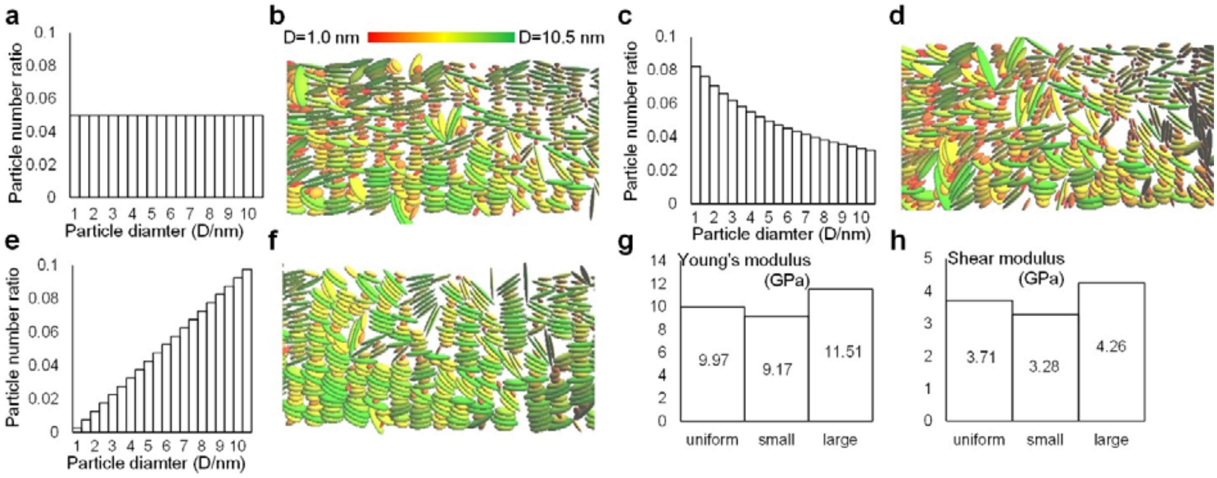

Figure 1 **a c e** Bar charts showing the particle size distribution. Particle number ratio indicates the number of beads with certain sizes, for example, if number ratio of particle with 1-nm diameter is 0.05 and the total bead number is 900, the number of 1-nm diameter bead is 45. **b d f** Snapshots of the poly-dispersed systems after equilibration in uniform, small-bead and large-bead cases respectively. **g h** Two bar charts showing Young's modulus and shear modulus of the samples with different particle size distributions

3. CONCLUSION

The proposed coarse-grained model for C-S-H manifests that, in hardened cement, C-S-H with more large beads has better mechanical properties. Such result indicates that relatively large beads serve as the major load-bearing constituent in C-S-H and hardened cement. The mechanical enhancement of cement could be achieved by increasing the portion of large particles. We envision that future studies could provide more physical insights in linking up hydration mechanism, microstructure and mechanical performance of cement.

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