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Dynamic mechanical behaviors of calcium silicate hydrate under shock compression loading using molecular dynamics simulation

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ABSTRACT

Dynamic mechanical behaviors of the calcium silicate hydrate (C-S-H) under shock compression loading in layered direction have been investigated by molecular dynamics (MD) simulations. The various piston velocities ranging from 0.2 to 3.0 km/s used to describe the propagation of stress waves have been employed in our MD simulations. The shock Hugoniot curve and the distribution of particle velocity are obtained. It is found that the Hugoniot elastic limit is 7.5 GPa, and the impact may induce elastic response, elastic-plastic response and shock regime. Our results reveal that only a continuous elastic wave exists when the particle velocity is below 0.5 km/s, while a new wave is generated when the particle velocity is at 0.5 km/s. With further increasing the particle velocity, a two-wave structure is generated. After the particle velocity is larger than 2.0 km/s, the shock wave is dominant. These findings provide important atomic insights for understanding the dynamic mechanical behaviors of C-S-H.

1. Introduction

Calcium silicate hydrate (C-S-H) is the main hydration product of Portland cement, which is the most important binding phase of concrete and responsible for numerous important properties of concrete such as hardening, shrinkage, and creep [1–3]. To improve the performance of concrete and design a kind of high strength concrete with good durability, understanding the structure and mechanical properties of C-S-H is of great scientific and technological interest. However, it is still a challenge to study C-S-H in atomic level mainly due to the inherent disorder and compositional variance of C-S-H [4–6].

Murray et al. [7] compared the mechanical properties of Hamid's 11 Å tobermorite structure [8] with a possible C-S-H structure constructed by the removal of the bridge tetrahedron in silica chain in 11 Å tobermorite. They found that when the silicate chain in C-S-H was discontinuous, the stress–strain curves for tension and compression are comparable to those at the macroscopic level. However, the generalizability of the C-S-H structure is limited, because there are some important features that are inconsistent with the actual structure. Based on the experimental data [6,9,10], Pellenq et al. [11] proposed a bottom-up atomic modeling method to construct the molecular structure of C-S-H. The mechanical stiffness, strength, and hydrolytic shear response of the molecular model were probed and compared to experimentally measured properties of C-S-H. Their results showed that the model can describe the general structure and compositional features of C-S-H, hence this model has be used to study elastic deformation and cracking. Meanwhile, by comparing the mechanical performance of dry and wet C-S-H, it was found that the large displacements of water molecules in wet C-S-H lowered the shear strength and resulted in unrecovered deformations during the loading process. Hou et al. [12,13] investigated the mechanical properties of the C-S-H during the axial stretching process in three different directions by using ClayFF force field [14], as well as the influence of the contained water percentage on the mechanical properties of the C-S-H by using the CSH-FF force field [15]. They have also investigated the crack evolution mechanism in the C-S-H by simulating the uniaxial tension test on the C-S-H with voids ranging from 0.5 to 5 nm [16]. Based on the model proposed by Pellenq et al., Qomi et al. [17] described a combinatorial approach to optimize properties of cement hydrates. In this approach, hydroxyl groups were introduced into the C-S-H model by modeling the chemical reaction of water molecules using ReaxFF force field [18–20]. Using the two C-S-H models with a calcium-to-silicon ratio (C/S) of ~1.67, the range of indentation modulus of C-S-H under CSH-FF force field between 60 and 70 GPa showed that the effect of hydroxyl groups

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on C-S-H model could be ignored in a certain degree. Bauchy et al. [21] used the ReaxFF force field to study the fracture toughness of C-S-H. Palkovic et al. [22] investigated the constitutive response of C-S-H under combined loading.

While many previous studies on C-S-H have mainly focus on molecular structure analysis and mechanical properties, few efforts have been made to investigate their dynamic mechanical properties under shock compression loading. Shock waves have been used to study the equation of state of materials under extreme conditions [23–25] and non-equilibrium atomistic simulations (NEMD) have proved to be a powerful tool to study shock wave propagation in solids [26,27]. The characteristic times in strong shock experiments can be achieved in MD simulation, making it possible to directly compare results between simulation with experiment [28,29]. Shock compression experiments usually use the combination of light gas gun with other instruments such as velocity interferometry, polyvinylidene fluoride stress gages, photonic doppler velocimetry system, and inclined mirror technique to measure the shock velocity (U_s), the particle velocity (U_p) and the stress [30,31]. Due to the difficulty in measurement of the pressure, the specific volume, and the internal energy, the U_s-U_p Hugoniot curve is the most commonly used in experiments. In contrast, MD simulations can get these variables easily and display the propagation of stress waves in details. Therefore, MD simulation can shed light on the atomic-level understanding of the mechanisms of shock wave [32]. The present study aims to investigate the dynamic mechanical behaviors of C-S-H subjecting to shock compression loading. In our MD simulations, the momentum mirror method [33] is employed to produce shock waves, by slamming the sample upon against a specular reflecting wall at a piston velocity.

2. MD simulation

2.1. Model and force field

MD simulation as a powerful tool [34,35] is used to study the dynamic mechanical response of C-S-H under dynamic shock loading via the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [36–38]. The layered direction, which consists of water layers and calcium-silicate layers and has the weakest tensile strength [13], is chosen to study the dynamic mechanical response of C-S-H under shock loading. The amorphous C-S-H model is constructed, following the procedures proposed by Pellenq et al. The ClayFF force file [14] is employed to describe the interatomic interactions between atoms in C-S-H. Periodic boundary conditions (PBCs) are imposed along all three dimensions. In order to obtain the C-S-H model, the supercell (4a × 3b × 1c) of Hamid's 11 Å tobermorite (C/S = 1.0), without water molecules and any hydroxyl group, is taken as the initial configuration of the C-S-H model.

Firstly, we convert the C-S-H model from monoclinic box into the orthogonal box, as shown in Fig. 1(a–b). During the conversion, the relative atomic position and model volume are unchanged. Particles located outside of the simulation cell are mapped back into the box by wrapping their coordinates around at the periodic boundaries of the simulation box. In addition, partial SiO_2 group in silica tetrahedron are deleted to satisfy the Q_n distribution [39] and the C/S ratio [6]. Then, the energy minimization with conjugate gradient (CG) algorithm is used to relax interlayer calcium atoms, and subsequently to all other atoms and the box dimensions. Water molecules are adsorbed into the dry disordered C-S-H structure using Grand Canonical Monte Carlo (GCMC) [40] at 300 K with 0.5 eV of the chemical potential which corresponds to normal liquid water at 1 g/cc and 300 K. Finally, the system is equilibrated at 300 K for 100 ps in an isothermal-isobaric (NPT) ensemble at zero external pressure.

The velocity Verlet method is used to integrate the classical equations of motion of particles with a time step of 0.1 fs. The calculated chemical composition and density of the C-S-H are $(CaO)_{1.67}(SiO_2)(H_2O)_{1.69}$ and 2.40 g/cm^3, respectively, which are in good agreement with the results obtained by the neutral scattering tests [6].

2.2. Computational details

The simulation samples are constructed by replications of the single cell shown in Fig. 1. The final C-S-H sample of dimensions of 7 (x) × 7 (y) × 110 (z) nm^3 which is large enough for the observation of the whole wave structures, is subjected to shock compression loading in z directions. For shock loading tests, PBCs are imposed along x and y directions to minimize the surface and edge effects. To analyze the propagation of stress waves and the dynamic mechanical properties of C-S-H, the particle velocity, stresses and density are calculated along the impact direction, and recorded in shock profiles with binning analysis. The Virial method and atomic Voronoi polyhedral volume are used to calculate the local stresses [41]. During the shock compression loading, the simulation is performed in the isochoric-isoergic (NVE) ensemble in order to exactly compute the microcanonical dynamics.

Along the z direction, the dynamic shock is loaded at one end of the super-cell by using a momentum mirror technique [33], as shown in Fig. 2. In the momentum mirror technique, the simulation is bounded with a moving wall which reflects particles and drives the system with an effective infinite-mass piston which is capable of driving shock waves. During shock compression loading, the simulate box is divided into evenly spaced bins with the width of 15 Å and physical quantities in each bin are obtained. Meanwhile, the other end of the simulate box is free boundary condition. In order to minimize the possible artifacts due to the moving wall on one end and the free surface on the other end, the atoms within the ends are excluded from the analysis.

3. Results and discussion

3.1. Shock Hugoniot pressure-specific volume (V = 1/ρ) curve

In order to find the Hugoniot elastic limit (HEL) which distinguishes a material transitions from a purely elastic state to an elastic-plastic state, the shock Hugoniot P-1/ρ curve shown in Fig. 3 is obtained by applying particle velocity from 0.2 to 3.0 km/s in the layered direction.

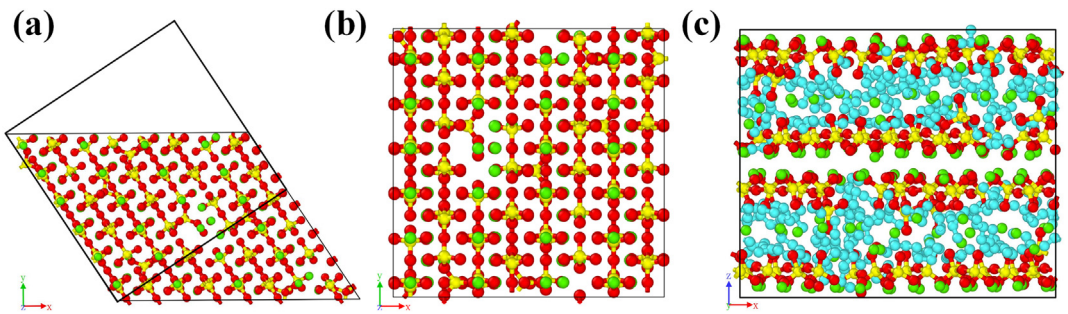

Fig. 1. Schematic diagram of the simulated C-S-H sample. (a) Original monoclinic cell. (b) Transformed orthogonal cell. (c) Final model of C-S-H.