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Study on Multi-Scale Tensile Strength and Tensile Strain of Calcium Silicate Hydrate Layered Nanocomposites Under External Physical Field

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Abstract

Calcium silicate hydrate (C-S-H) is the mainly strength source of cement-based materials, but there is little basic research. In this paper, molecular dynamics method is applied to analyze the multi-scale tensile strength and tensile strain of C-S-H layered materials under the condition of external physical fields (temperature and strain rate). The results show that the tensile strength and strain of C-S-H model decrease with temperature raises. The temperature (from 1 K to 600 K) has obvious influence on the tensile strain and strength of C-S-H layered materials. In addition, at (0.00025 ps^{-1}-0.001 ps^{-1}), the tensile strain and strength of C-S-H layered materials are less sensitive to strain rate. The whole model is closer to a 3-dimensional deformation. However, at (0.001 ps^{-1}-0.005 ps^{-1}), the dynamic load effect begins to increase, and the work done by the load per unit time increased. The tensile strain and strength of C-S-H layered materials indicates intensified by the change of strain rate. The energies are randomly distributed in the system, not concentrated in a certain area.

Keywords: *Hydrated calcium silicate; External physical field; Multiscale; Mechanical properties; Molecular dynamics*

1 Introduction

Cement-based nanomaterials are a one of the largest manufacturing material in the world. A terrible data for cement-based nanomaterials is put into buildings every year. It inevitably deepens the burden on the environment. About 5% of carbon dioxide (CO_2) emissions are produced by cement-based industry [1-4]. Therefore, it is necessary to decrease the amount of cement-based nanomaterials and to enhance the service life are the keys to realize "carbon neutrality".

Calcium silicate hydrate (C-S-H) is the mainly hydration product of cement-based nanomaterials, accounting for about 60-70% of the total product volume. It is generally considered as the key components that affects the service life of cement-based materials [5]. However, the C-S-H layered nanostructure is only maintained by van der Waals force and weak ionic bond. Therefore, how to control and improve the service life of C-S-H is the frontier direction of preparing high performance concrete.

Scholars have been committed to the characterization and basic performance research of C-S-H layered nanostructure [6]. However, complex chemical composition and microstructure of C-S-H layered nanostructure are still controversial [7].

Atomic/molecular scale first-principles calculation and molecular dynamics (MD) are applied to understand the dynamic modes of complex chemical systems from different physical levels [8].

Multi-level structure and interface design has been confirmed an effective way to improve the performance of engineering structural nanomaterials.

The C-S-H models were established by MD. The multi-scale tensile strength and tensile strain of C-S-H layered nanostructures under different temperature are studied.

The relationship between tensile strain and tensile strength of C-S- H layered composites and different temperatures were analyzed. In addition, the tensile strain and tensile strength of C-S-H layered nanostructures with different strain rates were studied by MD. The tensile strain rate dependence of C-S-H layered nanostructures was analyzed.

2 Models and Methods

The initial model of C-S-H is constructed based on the crystal structure of 11 Å Tobermorite. Some water molecules in the crystal model were removed. The

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calcium-silicon skeleton structure [11-12] was obtained, as shown in Figure 1.

Some calcium ions were added at the same time, so that the final polymerization degree distribution of the silicon-oxygen tetrahedron met the results of NMR test [13].

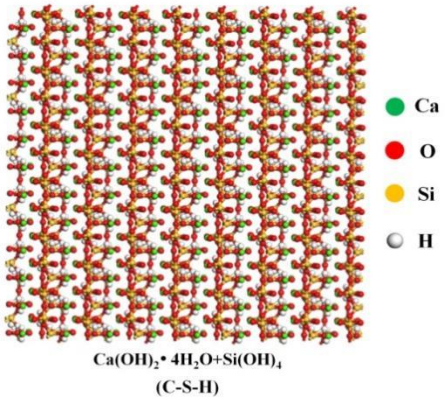

Figure 1 Initial models of C-S-H. Spheres with green, yellow, white and red represent calcium, silicon, hydrogen and oxygen atoms.

The force field of ReaxFF in LAMPS software [14-15] is applied to simulate the tensile strength and strain of C-S-H models [16]. The ReaxFF can accurately simulate the covalent and electrostatic interactions of various materials. The Equation (1) can be described as:

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{lp} + E_{val} + E_{tors} + E_{Coulomb} + E_{vdW} \quad (1)$$

Where E_{bond} are the energies related to the formation of bonds between atoms, E_{over} and E_{under} are correction terms based on valence rules to prevent atoms from over-coordinating and under-coordinating, respectively. E_{lp} is a lone pair event. E_{val} and E_{tors} are energy related to valence angular strain and torsional angular strain, respectively. $E_{Coulomb}$ and E_{vdW} are non-key items.

The Verlet algorithm are applied to measure the atom trajectory in the simulation. The time steps are set to 0.25 fs. Then, 50 ps is relaxed in the NPT ensemble, so that the kinetic energy, potential energy and temperature of the system reaches balance. Finally, MD system are measured by using 0.001 ps^{-1} of tensile loading.

3 Results and Discussion

3.1 Mechanical properties of C-S-H model

The stress-strain curves of C-S-H models at the condition of temperature 300K are display in Figure 2. Obviously, the three situations are found in tensile deformation of C-S-H models, including (ε=0-0.005 elastic region), (ε=0.005-0.118 plastic region) and (ε>0.118 fracture region). In the elastic region, the tensile strength and strain of C-S-H models increases linearly with adding tensile strain. As tensile strain continues to increase, the stress no longer increases linearly with the strain, that is, it exceeds the allowable values of tensile deformation of C-S-H models and enters the plastic stage. At this time, the peak stress is 1.068 GPa. The plastic strain increases sharply when external loading exceeds the limit threshold. In addition, it is known from the stress-strain curves that C-S-H model has no obvious yield platform in the process of tensile deformation. From the perspective of micro-level chemical bonds, the C-S-H layered nanostructure is maintained only by weakly ionic bonding and vdW force, which shows brittle fracture. C-S-H is one of the main sources of concrete strength. From the perspective of fracture mechanics, it is also confirmed that macro concrete has the characteristics of brittleness and poor toughness.

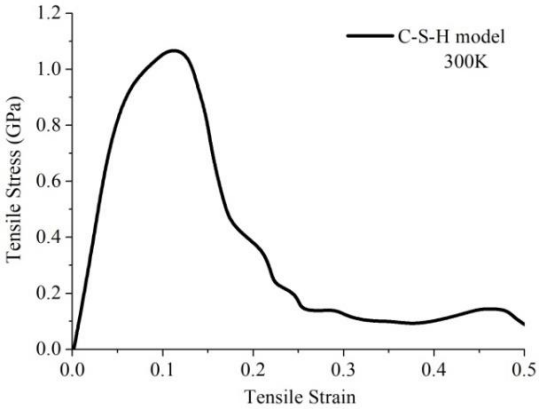

Figure 2 Stress-strain curves of C-S-H model at 300 K.

3.2 Temperature dependence of mechanical properties of C-S-H model

The hydration speed of cement-based nanomaterials also changes with the change of temperature. With the increase of temperature, the reaction is faster, showing strong temperature dependence. [17]. In order to fully consider the dependence of mechanical properties of C-S-H layered nanomaterials on temperature, the dependence of tensile strain and strength of C-S-H layered nanomaterials on temperature change was measured in the thermodynamic temperature range of [1 K, 600 K]. Figures 3(a) and 3 (b) show the tensile strain and strength of the C-S-H model at different temperatures (1 K, 150 K, 300 K, 450 K and 600 K) respectively.

When the temperature rises from 1 K to 600 K, the tensile strain and strength of C-S-H model decrease. The tensile strain of C-S-H model decreases from 0.137 to 0.081, with a decrease of 40.87%. However, the tensile strength and strain of C-S-H model decreases by 50.21%. Compared with tensile strain of C-S-H model, tensile strength of C-S-H model are more sensitive to the change of temperature.

From the foregoing, the tensile strain and tensile strength of C-S-H model have high correlation on temperature. The kinetic energies-related temperature can be described by using the formula [18]:

$$E_p = \sum_{j=1}^{N} \frac{1}{2} m_j v_j^2 = \frac{3}{2} N k_b T \quad (2)$$

Where E_p is the total kinetic energies, N indicates the number of atoms of simulated model, T represents the temperature and k_b is the Boltzmann constant.

Obviously, the total kinetic energies of C-S-H model increases with the increase of temperature. When adding temperature, the vibration amplitude of atoms in the C-S-H model increases at their equilibrium positions. It leads to the relative decrease of the mutual attraction between atoms in the model. These atoms in the C-S-H model easily escaped from their original positions. When the C-S-H model is subjected to external load, it will cause the lattice to expand and break through. In addition, these atoms are in a "semi-activated state", which makes them more likely to exceed the constraints of binding energy.

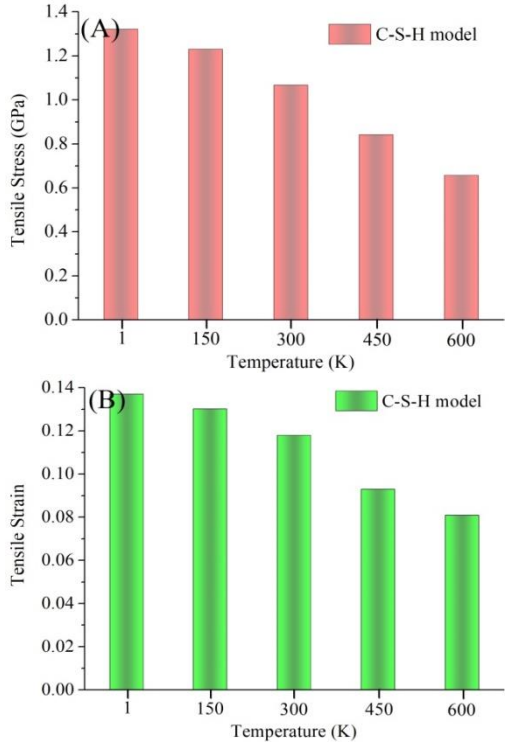

Figure 3 Mechanical properties of C-S-H model at different temperatures (1 K, 150 K, 300 K, 450 K and 600 K). (a) the tensile stress of C-S-H model and (b) the tensile strain of C-S-H model.

3.3 Strain rate dependence of mechanical properties of C-S-H model

In order to fully consider the effect of strain rate on the tensile strain and strength of C-S-H layered nanomaterials, the dependence of tensile strength and tensile strain of C-S-H layered materials on strain rate changes was measured in five strain rate ranges ($0.00025ps^{-1}$, $0.005\ ps^{-1}$, $0.001ps^{-1}$, $0.0025ps^{-1}$ and $0.005ps^{-1}$).

Figure 4 indicates the tensile strain and tensile stress of C-S-H layered materials at different strain rates. It is found that tensile strain and tensile stress increase with the increase of strain rate. There is a critical strain rate for the tensile strength and strain of C-S-H layered materials, which is about 0.001 ps^{-1}. At low strain rate (0.00025 ps^{-1}-0.001 ps^{-1}), the tensile stress and strain of C-S-H layered materials have no obvious change. Meanwhile, the mechanical properties of C-S-H layered materials are insensitive to the strain change rate. However, at high strain rate (0.001 ps^{-1}-0.005 ps^{-1}), the change of strain rate has obvious influence on the tensile stress and strain of C-S-H layered materials. The tensile stress and strain of C-S-H layered materials are significantly dependent on the change of strain rate during the tension process.

When the strain rate is less than the threshold, C-S-H layered nanomaterials have many opportunities to consume the energy of tensile deformation, so their positions can be redistributed to adapt to stress concentration. This makes the whole model tend to be balanced and closer to quasi-static tensile deformation. The energy cannot be uniformly distributed in the whole system, so it can absorb more energy and obviously increase its strength.

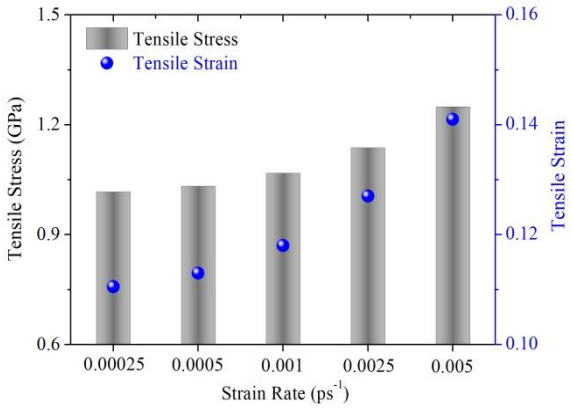

Figure 4 Tensile stress and strain of C-S-H model at different strain rate (0.00025 ps^{-1}, 0.0005 ps^{-1}, 0.001 ps^{-1}, 0.0025 ps^{-1} and 0.005 ps^{-1}).

4 Conclusion

MD method is applied to study and analyze the multi-scale tensile strength of C-S-H layered materials under the action of external physical fields (temperature and strain rate). The results show that the tensile strength of C-S-H model decreases with the increase of temperature. The temperature (from 1 K to 600 K) has obvious influence on the tensile strength and strain of C-S-H layered materials.

When the temperature rises, these atoms are in a "semi-activated state", which makes them more likely to exceed the binding energy constraints. In addition, at low strain rate (0.00025 ps^{-1}-0.001 ps^{-1}), the whole process is closer to quasi-static loading. The energy distribution of the whole system is uniform.

The energy difference of individual atoms is very

small, and the time and chance for each atom to reach or even exceed its energy threshold are equivalent. Therefore, the tensile stress and strain of C-S-H layered materials have little change, showing little sensitivity to strain. However, at high strain rate (0.001 ps^{-1}-0.005 ps^{-1}), C-S-H layered materials will experience high energy density in a short time. The time for uniform dissipation of external load will be reduced. It shows the great changes and strong correlation in tensile stress and strain.

Declarations

Conflict of interest: The author did not report a potential conflict of interest.

Informed consent: I assure you that this manuscript has not been submitted for publication elsewhere.

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