



Enhancing the interfacial bond strength of cement nanocomposite with carbonate nanostructure



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ABSTRACT

The future development of cementitious materials with nanoparticles or nanoscale fibers requires the ability to understand and to improve the interfacial bonding in order to develop a stronger, tougher and more robust concrete nanocomposite. The purpose of this work is to study the adhesion contact as well as the interfacial strength between calcium silicates hydrates gel (C-S-H) and calcite surfaces. The application of lateral and longitudinal strain on both surfaces shows that the elastic energy of C-S-H to ensure accommodation at the interface is lower than the one obtained for calcite. Our results show that 1 Å is the ideal distance to have a good adhesion between (001) C-S-H and (104) calcite surfaces. We also demonstrate that the presence of water molecules at the interface absorb the excess energy and thus contribute to the stabilization of the interface. Besides, the results indicate that the interfacial bonding between C-S-H and calcite improves the ductility of the cement nanocomposite when the gel porosity is about 30%. Under uniaxial and shear stresses, the nanostructure shows a heterogeneous mechanical behavior. Particularly, the interfacial shear strength enhances while applying a shear stress, which is due to the structure and the dynamic differences of the layered structure since the calcium silicate layer, constructed by Ca–O and Si–O ionic-covalent bonds, has stronger cohesive force than the interlayer H-bond network.

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1. Introduction

Macroscopic mechanical properties of cement-based nanocomposite are improved through reinforcing its microstructures at a microscopic level, which is actually a real challenge for scientists. Thanks to nanotechnology developments, research may have the potential to engineer concrete with superior mechanical properties through the use of nanoparticles. There are four reasons that the incorporation of nanoparticle has a strong influence on the mechanical properties of concrete: the high surface area that provides high chemical reactivity, the size of C–S–H gel diameter (~10 nm) which permits to the dispersed nanoparticles to fill voids resulting in denser concrete, the high reactivity of nanoparticles which accelerate cement hydration and the pozzolanic reaction to react with Ca(OH)₂, producing an additional quantity of C–S–H gel.

Experimental studies show the effect of nano-sized mineral additions on ductility of engineered cementitious composites (ECC)

containing high volumes of fly ash at different hydration degrees [1–14]. Results confirmed that mineral additions could significantly improve both flexural strength and ductility of ECC, especially at early ages. S. Yeşilmen et al. [14] demonstrate that nano-sized CaCO₃ was cheaper and a successful mineral to improve the flexural deformation capacity of ECC [14]. Experimental measurements [15] indicated that the use of nano-CaCO₃ accelerate the hydration rate of cement. It could be explained that a mass of C-S-H gel formed and the density degree of hardened cement paste increased.

On the other hand, fundamental research on the mechanical properties of CaCO₃ whisker-reinforced Portland cement has been carried out by Cao et al. [16] shows excellent mechanical properties. In more recent studies [17], calcium carbonate whiskers have been proposed as a kind of micro-reinforcement in cement based composites. The addition of whiskers decreases the brittleness of cement-based composite, delays the formation and propagation of microcracks. In Fig. 1 is presented the microstructures of hardened cement with/without whiskers. They demonstrate that the addition of CaCO₃ whiskers led to a relative compact microstructure of

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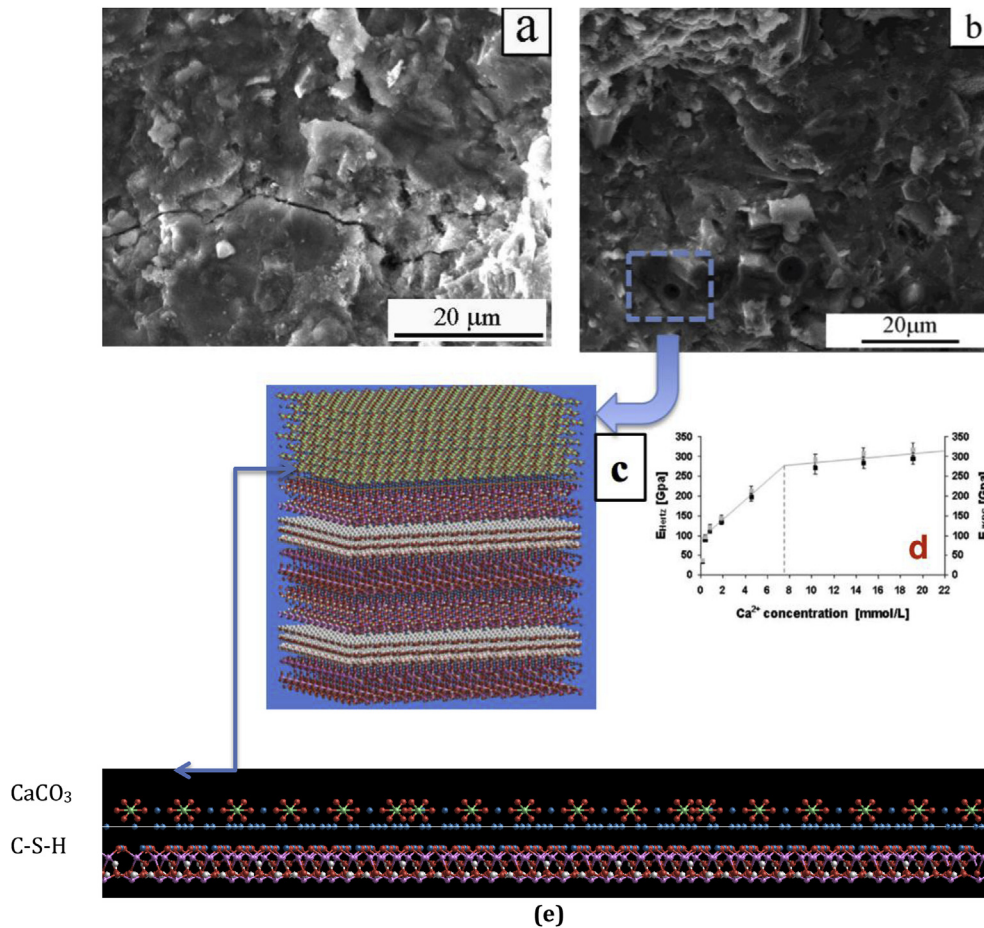


Fig. 1. Microstructures of hardened cement (a) without whiskers and (b) with whiskers [16,17]. (c) Atomistic structure of C-S-H/calcite nanostructure. (d) Evolution of the elastic modulus with concentration of calcium hydroxyl [64]. (e) Atomistic configuration of the (001) C-S-H/(104) CaCO_3 interface.

hardened cement. Their results show that the micromechanical mechanism is strongly related to the bonding properties between whiskers and cement matrix. Brarathi et al. [18] prove in their experiments that calcium carbonate precipitating enhance the chemical properties of cement concrete. Although CaCO_3 whiskers can reinforce cement-based composites at the microscopic level, there is still a main problem need to be solved: the measurement of the interfacial bond strength between CaCO_3 surface area and cement matrix. Appropriate interfacial bond strength is advantageous to achieve the best strengthening and toughening effect.

The purpose of the present research is to explore the interfacial bond strength of cement nanocomposite consolidated by carbonate and to explain how can we enhance it. Using molecular dynamics simulation method, we will analyze at the nanoscale level the fundamental interactions between CaCO_3 and C-S-H gel, the main constituent of cement paste. We note that this computational method was widely used for calcite [19–30] and C-S-H gel [31–35].

We particularly study, here, the technical connection between the (104) calcite and (001) C-S-H surfaces, as well as the conditions to get a stable assembly. To this end, the appropriate force field is used to describe the bonding character at the interface. We will focus on the structural and energetic properties at the interface, evaluate the lattice mismatch between the two compounds, the adhesion energy, the work of separation as well as the elastic energy at the interface. We will examine the mechanical behavior of the C-S-H/ CaCO_3 nanocomposite under normal and shear stresses.

2. Description of the structure and the bonding at the interface of C-S-H/ CaCO_3 nanocomposite

In the present work, we have used Hamid's model [36] to describe one grain of C-S-H as a tobermorite 11 Å layered structure ($\text{Ca}_5 [\text{Si}_6\text{O}_{16}(\text{OH})_2] 2\text{H}_2\text{O}$). Besides, we have used the slit-pore model, in which two grains of C-S-H are separated by an intergranular pore of 1nm^{35} . Water is present in the interlamellar spaces as well as in the intraglobular pores. The atomic coordinates, crystal parameter and space group were obtained from XRD data and other literature [37–39]. The coordinates of hydrogen atoms for all the hydroxyl and water molecules were derived from the atomic positions of the oxygen atoms. The hydrogen atoms are located at about 1 Å from the oxygen atoms of hydroxyl and water molecules. In the case of water, H-OH angle corresponds to 109° . Regarding CaCO_3 , we have used the most stable phase, which is calcite. Therefore, C-S-H/ CaCO_3 interface is constructed by considering the stable surfaces of both (001) C-S-H and (104) calcite. Then, we have built a supercell by extending the unit cell of C-S-H (tobermorite 11 Å) 3 times in the x direction and 11 times in the direction. For CaCO_3 , we have duplicated the unit cell 4 times along x-axis and 3 times along y-axis. Then, we put the (104) surface of CaCO_3 , terminated by $\text{Ca}^{2+}\text{CO}_3^{2-}$ atoms, on the top of the (001) C-S-H surface terminated by Ca^{2+} atoms (Fig. 1 e). The obtained simulation box is of $(2.01 \times 7.40 \times 9.10)$ nm, containing calcium carbonate atoms in contact with those of C-S-H (Fig. 1 (c)). The gap distance between calcite and C-S-H atoms is varied from 0.5 to 3 Å. We

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