



Design of a novel nanocomposite with C-S-H@LA for thermal energy storage: A theoretical and experimental study

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HIGHLIGHTS

- C-S-H@LA nanocomposite was firstly prepared.
- Some novel design rules for PCM fabrication were offered both experimentally and theoretically.
- C-S-H@LA was experimentally characterized as a promising material for TES.
- The melting behavior was theoretically investigated via molecular dynamics.

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ABSTRACT

In this work, emphasis was placed on the design of a novel nanocomposite for thermal energy storage in the field of green building constructions. Calcium silicate hydrate (C-S-H), the primary product of cement hydration, was firstly introduced as mesoporous accommodations for lauric acid, from an experimental and theoretical perspective. In detail, C-S-H@LA composite was systematically examined through experiments, in terms of Scanning Electron Microscope, Transmission Electron Microscope, Brunauer–Emmett–Teller gas sorptometry, Fourier Transform Infrared Spectroscopy and Differential Scanning Calorimeter. Results demonstrated C-S-H@LA was one promising composite PCM with 32.04 kJ kg^{-1} latent heat capacity, $0.514 \text{ W m}^{-1} \text{ K}^{-1}$ thermal conductivity and 91.04% energy storage efficiency. No chemical bonds were found between C-S-H and lauric acid. Notably, stability of C-S-H@LA embracing structural, chemical and thermal properties were also verified. Innovatively, molecular simulation was applied to explain the melting behavior of C-S-H@LA that could be divided into three stages, i.e. acceleration period, stationary period and secondary rising period, based on diffusion coefficient. This work has emerged some new design rules for PCMs fabrication.

1. Introduction

In recent years, thermal protection and insulation have been two important issues encountered in many fields such as agricultural, medical and industrial [1]. These two problems have raised great attention and been popularly considered for sustainable development. Among thermal energy storage (TES) systems, latent heat storage based on phase change materials (PCMs) is a particularly attractive technique because of high latent heat storage density and small temperature variation [2–4]. Considering the desirable properties, thermal energy storage materials have been widely used for efficient energy management and utilization in terms of solar energy storage [5–7], battery

thermal management [8] and building energy conservation. Generally, it is efficient to incorporate PCMs into building fabrics by either integrating them into construction materials or using them as components [9,10]. Consequently, a consensus has been reached that strategy of latent heat storage is extremely potential in thermal resistance of building elements, such as concrete walls, floors, and roofs.

Application of PCMs as composites has been acknowledged as a promising technology and proposed as one method of energy saving for buildings [11]. In the field of construction materials, some porous materials like natural minerals have been widely used as carriers or fillers to absorb and release heat [4]. Lv et al. once investigated kaolin incorporated paraffin via vacuum impregnation method [12]. Their

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results indicated that this kind of composites has a high thermal conductivity ($0.413 \text{ W m}^{-1} \text{ K}^{-1}$) and a huge latent heat capacity ($119.49 \text{ kJ kg}^{-1}$). Additionally, researches on intercalated and micro-encapsulated PCMs have been subjected to considerable interest in the last two decades [13–15]. Considering the high efficiency, such PCMs could be practically used in buildings as TES concrete to reduce energy consumption. For example, utilization of PCM impregnated gypsum wallboard has a significant effect on room temperature adjustment, by declining about 4°C during the day and reducing the heat load at night. Similar applications were also carried out by Hunger [15], Xu [16] and etc. It should be noted that these PCMs showed excellent thermal impact on energy storage. However, when PCMs are applied in these manners, there inevitably remain some problems in terms of cost, operation and compatibility. Firstly, it should be put at the very best place to notice the limited reserves of natural clay, including perlite and diatomite, which bring about higher cost. Secondly, purification and even future functionalization and group modification are also needed, considering the impurities in these natural minerals [17]. Finally, there still exist some incompatibility problems between PCMs and cement matrix [18], which reflects as a decreased compressive strength and thermal capacity owing to the weak bonding behaviors between the two.

Researchers tend to discover some natural minerals, such as dolomite, diatomite and etc. to fabricate as composite PCMs. Compared with such natural minerals, calcium silicate hydrate (C-S-H) is recognized as a renewable and recycled resource, which is an ordinary construction material and binding phase of Portland cement paste [19]. Generally, Portland cement concrete is the world's most widely used manufactured material, with more than 11 billion metric tons consumed each year. It is such a normal material that some extraordinary properties and applications are usually neglected. According to the theory of Jennings [20], C-S-H comprises small nanoparticles in 5 nm average diameter, and forms a gel-like network. This indicates C-S-H is sorts of a 3D porous structure and conducive to the adsorption of PCMs [21]. Besides, preparation of C-S-H is quite simple and replicable. Only by mixing water and cement, then the C-S-H particles will cluster in nanoscale, relieving the fussy sample fabrications. As the main product of cement hydration, the compatibility between C-S-H and cement based matrix is positive for building constructions. Considering these superior properties of C-S-H, it could work as an alternative for PCM accommodation.

Another issue is the development in material simulation. Some simulation methods, especially molecular dynamics, have opened up a completely new path for material design. Based on molecular simulations, it is no longer the case that researchers had to blindly compound two materials for composite PCMs. Material design could be achieved based on properties and performances, which eliminates cumbersome experiments and interprets the mechanism of energy storage from a deeper perspective.

This work was inspired by some ordinary constructing materials like the most basic cement hydration products, C-S-H, to design a nanocomposite for TES in green buildings. Performance of this nanocomposite was verified by experiments and the mechanism of energy storage was analyzed using molecular dynamics. Basically, C-S-H was firstly introduced into PCMs, cooperated with lauric acid (a fatty acid), to the best of our knowledge. In detail, preparation and characterization of C-S-H@LA were carried out, covering hydration process, vacuum impregnation, morphology analysis, pore structure and thermal stability. Innovatively, molecular simulation was applied to design and elucidate this nanocomposite in atomistic scale. Emphasis was placed on the construction of C-S-H@LA molecular model to meet the practical requirements, embracing melting/freezing processes, melting temperature and etc. To sum up, we provided some new insights to design PCMs from atomistic scale both experimentally and theoretically thus it enriched the application of C-S-H in the field of TES.

2. Experimental details

2.1. Materials

Calcium nitrate ($\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$, 99%), sodium metasilicate non-anhydrate ($\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$, 99%), sodium hydroxide (NaOH, 96%) and lauric acid ($\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$, 98%) were purchased from Sinopharm Chemical Reagent Co., Ltd. All these chemicals were used as received without further purification. Millipore water ($\Omega > 18 \text{ M}\Omega \text{ cm}$, 25°C) and ethanol (99.7%) were used throughout.

2.2. Methods

2.2.1. Preparation of C-S-H

Solutions of calcium nitrate, sodium silicate and sodium hydroxide were prepared in decarbonized water according to the Kumar [22]. To be detail, C-S-H was synthesized by gradually adding calcium nitrate solution (1 mol L^{-1}) with continual stirring under nitrogen atmosphere to sodium silicate solution. The nominal Ca/Si molar ratio was 1.9 for C-S-H. Notably, pH value was kept between 13.1 and 13.3 by adding NaOH during the precipitation of C-S-H.

After aging suspension at 60°C for 24 h with continuous stirring, the precipitates were collected and separated by vacuum filtration over a 22 nm organic filter and later washed with ethanol and CO_2 -free deionized water to remove salts and unwanted ions. The precipitates were then washed with ethanol and dried at 70°C in a vacuum oven for 48 h. Particle size analysis was carried out and the average size of C-S-H nanoparticles is $6.67 \mu\text{m}$ shown in Fig. 1.

2.2.2. Preparation of C-S-H@LA

As illustrated in Fig. 2, after the synthesis of C-S-H nanoparticles, lauric acid molecules were intercalated into the porous structure of C-S-H in specific procedures. Briefly, C-S-H@LA composite was prepared by direct impregnation method in vacuum state. Firstly, C-S-H and lauric acid powders were dry mixed together in a mass ratio of 1: 3. Then C-S-H and LA mixture was processed at 80°C for 6 h in a vacuum drying oven. Finally, the C-S-H@LA composite was cooled down to room temperature for further characterization.

2.3. Characterization

The particle size distribution was measured by laser diffraction particle size analyzer, a Microtrac S3500 instrument. The distribution was determined in a wet operation mode (analytical grade ethanol as the dispersant at room temperature), in the resolution of $0.04 \mu\text{m}$.

The morphology of C-S-H and C-S-H@LA was investigated by scanning electron microscopy (SEM, FEI SIRION-100) and transmission electron microscope (TEM, Tecnai G2 20). Namely, the samples of SEM were prepared as follows. The samples were dried at room temperature and stuck onto copper type as powders, on an aluminium SEM stub. Moreover, the accelerated voltage was 20 kV and images were detected

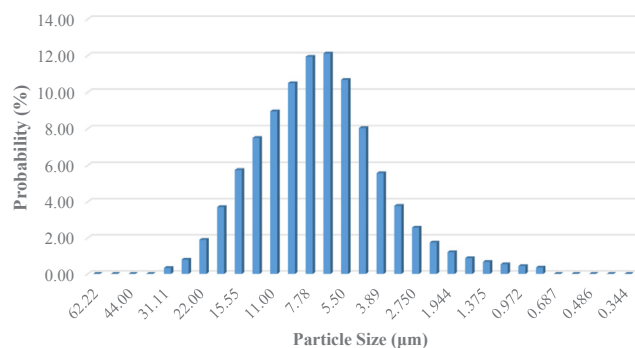


Fig. 1. Particle size distribution of synthetic C-S-H nanoparticles.

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