Study on crystallization behavior of fatty acids as phase change energy storage materials

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Abstract

Molecular arrangement of CA and MA, the eutectic composition and temperature of fatty acid binary mixtures CA-MA, and crystallization behavior of CA-MA (e.g., melting and crystallizing points, fusion heat and crystallization heat) are observed by intermolecular force, binary phase diagram, and DSC. The study shows that long-chain CA and MA molecules are arranged in bilayer structures with headgroups aligned next to each other. The eutectic composition of CA-MA is CA74.73MA25.27. The melting points and fusion heat, the crystallizing points and crystallization heat of eutectic mixtures are 21.80°C and 177.1J/g, 18.24°C and 172.6J/g, respectively. CA-MA has suitable phase change temperature and higher phase-change enthalpy. So, CA-MA can be used as the phase change energy storage material for building.

Keywords

Phase change material, Fatty acid, Capric acid, Myristic acid.

1. Introduction

Fatty acids have been reported as a most promising phase change material (PCM) because of the following advantages: renewable, suitable phase change temperature, high latent heat of fusion, non-toxicity, non-flammability, non-undercooling, no or little volume change, good thermal reliability after a large number of melting/solidification cycles, as well as compatible with many holding materials [1-3]. However, some drawbacks limit the application of the fatty acids to a large extent, such as the fixed phase change temperatures [4-5]. The eutectic mixture is a kind of composite which is composed of two or more components and each of them melts and freezes at the same temperature. The eutectic mixture has good thermal reliability. In this paper, PCM is developed based on fatty acid eutectics, aiming to solve the suitable phase change temperature of fatty acid and make it suitable to be incorporated in building materials. The fatty acid eutectics are prepared from Capric acid (CA) and myristic acid (MA). Various mass ratios are investigated to achieve the suitable phase change temperature by studying crystallization behavior of fatty acids.

2. Experimental

2.1 Materials

Decanoic acid (CA) and myristic acid (MA) are purchased from Sinopharm Chemical Reagent Co., Ltd.

2.2 Crystallization observation

Crystallization observation is carried out using a DSC Q2000 differential scanning calorimeter (TA, USA). 5-15mg of samples is added to aluminum sample pans under N2 flow of 80 ml/min, at cooling rates of 5 °C/min and interval of temperature of 80 -20 °C.

3. Results and discussion

3.1 Molecular structure

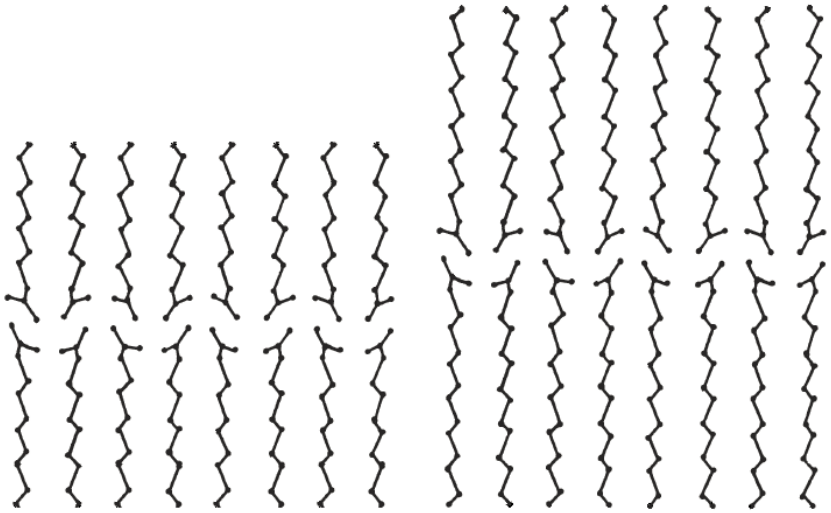
CA and MA are fatty acid (FA). They are aliphatic, straight chain, monocarboxylic acids. According to hybridized orbital theory, C–C carbon atoms from fatty acid (FA) are hybridized by equivalent SP3. These four SP3 hybridized orbitals take the shape of a regular tetrahedron with included angle of 109.5°. Therefore, the carbon atoms of alkyl in CA and MA are arranged in straight lines and zigzags at included angle of 109.5°. The molecular structure of CA and MA are shown in Fig. 1.

(a) CA (b) MA

Fig. 1 The molecular structure

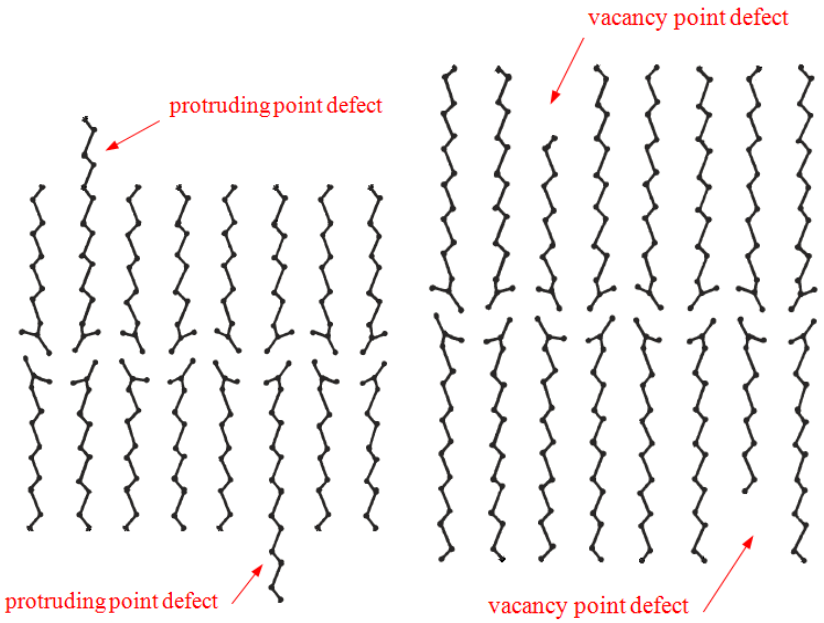
3.2 Molecular arrangement

The long-chain fatty acids molecules possess sufficient polarity in the carboxylic headgroup, giving them an amphiphilic nature and allowing the formation of bilayer structures with headgroups aligned next to each other inside the crystal and away from nonpolar bulk liquid. Crystal stacking structure schematic diagrams of CA and MA molecular are as shown in Fig.2.



(a) CA (b) MA

Fig.2 Crystal stacking structure schematic diagram



(a) Protruding point defect (b) Vacancy point defect

Fig.3 Crystal stacking structure schematic diagram of CA-MA

CA blending with MA can formed point defect of crystal stacking structure, see Fig.3. CA blending with MA can formed point defect of crystal stacking structure, see Fig.3. These point defects become the active sites of crystal growth to form a eutectic mixture, decrease crystallization temperature.

3.3 Crystallization

Binary phase diagram of CA and MA is illustrated in Fig. 4. The eutectic composition of CA-MA is 74.73w% (CA). The eutectic temperature Teu of CA-MA is 23.61°C. The phase transition enthalpy is 154.06 J/g.

The DSC of CA74.73MA25.27 is shown in Fig.5. From Fig. 5, the temperature of melting and crystallizing are 21.80 and 18.24°C respectively, and fusion heat and crystallization heat are 177.1 and 172.6J/g. So CA74.73MA25.27 can be used as a phase change energy storage material for building.

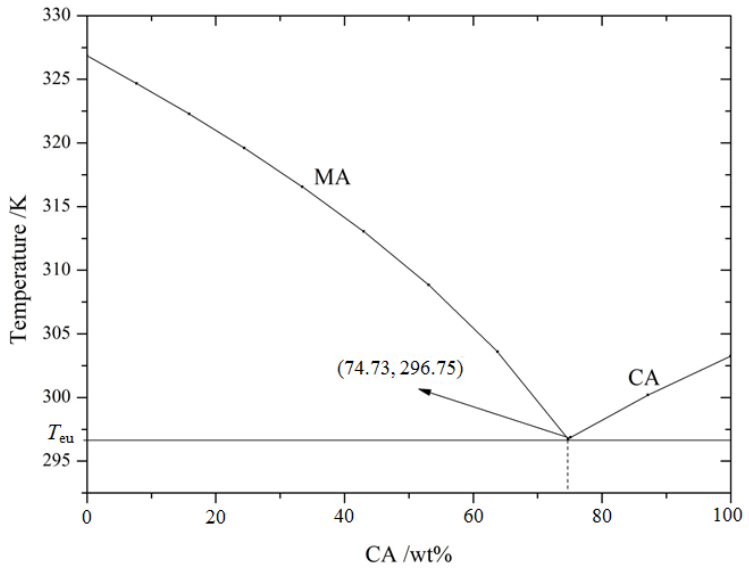


Fig. 4 Binary phase diagram of CA-MA

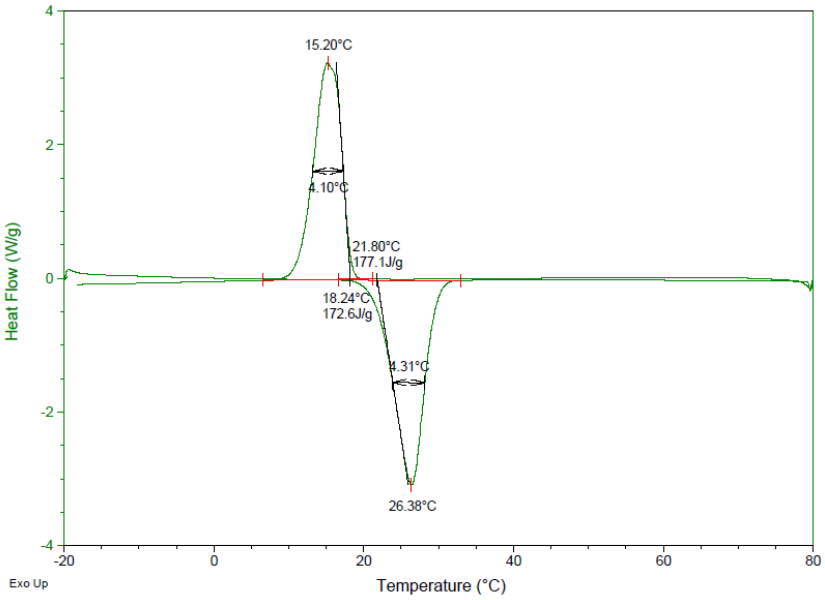


Fig.5 The DSC curves of CA-MA

4. Conclusion

Based on the results of this study, we conclude that:

Molecular arrangement of long-chain CA and MA molecules are stacked together side-by-side of bilayer structures with headgroups aligned next to each other. CA blending with MA causes the formation of crystal protruding and vacancy point defect, form a eutectic mixture, and decreasing crystallization temperature to 23.61°C.

The melting and crystallizing temperature of CA74.73MA25.27 are 21.80 and 18.24°C respectively, fusion heat and crystallization heat are 177.1 and 172.6J/g. It can be used as a phase change energy storage material for building.

Acknowledgements

This research was supported by Anhui Provincial Natural Science Foundation (1408085ME109) and National College Students' innovation and entrepreneurship training program project (201610361059).

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