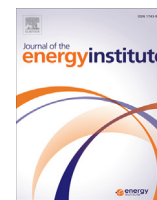




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Diffusion and thermal conductivity of the mixture of paraffin and polystyrene for thermal energy storage: A molecular dynamics study

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ABSTRACT

The development of thermal energy storage material is of vital importance to relieve the severe challenges of energy crisis. Phase change material and microencapsulated phase change material for energy storage is an important branch of thermal energy storage technology. In this paper, the simplified amorphous cell model was constructed with n-octacosanoic ($C_{28}H_{58}$), n-docosane ($C_{22}H_{46}$) and polystyrene (PS), which was used to investigate the heat and mass transfer of this system by performing molecular dynamics (MD) and non-equilibrium molecular dynamics methods (NEMD). The simulation results showed that the self-diffusion of this system will enhance with increasing temperature. Furthermore, higher temperature contributes to the extension of catenulate molecules, especially for polystyrene, which actually enhances the mass transfer of system. In addition, the thermal conductivity of the system increases with continuously increasing temperature, but the values are lower than that of pure paraffin. Therefore, the high thermal conductivity additives are required to be added into the mixture in order to improve the ability of heat transfer of the material.

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1. Introduction

It is inevitable to develop thermal energy storage technology to mitigate the energy crisis and reduce environmental pollution. Among a variety of thermal energy storage technology, phase change materials (PCM) for the excellent ability of heat storage has been widely investigated and gradually applied in the industrial fields [1–4]. Unfortunately, only several kinds of phase change materials can become candidates for practical applications because of their inherent shortcomings, for example, the low thermal conductivity, bad compatibility with the plastic device and flammability of organic compounds and the undesirable stability of inorganic compounds [5]. To get over these undesirable disadvantages, tremendous efforts have been made by scientific researchers in the past decade. Microencapsulated phase change materials (MEPCM) which are usually fabricated by PCM core and organic or inorganic shell have attracted wide attentions. The MEPCM can avoid PCM's leak after melting, prevent to corrode containers and be also used in the nanofluid field. Nowadays researches about MEPCM are mainly focused on the experimental preparation and characterization of the material properties. For constructing the core-shell structure of MEPCM, the preparation methods basically include in situ polymerization, interfacial polymerization, suspension-like polymerization and complex coacervation [1]. Among various core materials, paraffin of which main component is straight chain alkanes, owing to its superiorities [6] such as high latent heat, almost no supercooling, low vapor pressure when melts, no phase separation and cheap, is suitable for the core material of most MEPCM [7–11]. The shell materials are usually various organic polymers such as polystyrene [12–14], polymethylmethacrylate (PPMM) [15], urea and formaldehyde [16], in particular, a few inorganic materials such as silica [17] can also be used to encapsulate core materials. Moreover, researchers alter and optimize specific experiment process, change certain materials and add heat transfer enhancement materials to improve the performance of MEPCM.

However, the literatures that investigated the mechanisms of heat and mass transfer or simulated thermal physical properties of MEPCM from microcosmic or mesoscopic perspectives are relatively few. Only our group studied MEPCM by utilizing molecular dynamics and dissipative particle dynamics (DPD) methods, which are research methods of micro level and mesoscopic level, respectively. The superiority

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of MD or DPD is the different perspective from the macroscale experiment, which can investigate the deeper mechanism by analyzing the microcosmic or mesoscopic structure dynamic change and characteristic. There is no doubt about the difficult to achieve this by experimental methods.

In our previous works, the molecular dynamics method was performed to investigate melting mechanism and self-diffusion of MEPCM that were fabricated with the n-octadecane as core material and soft/hard SiO₂ structures as shell material [18]. After that, previous work was extended to study the heat and mass transfer mechanisms of abovementioned MEPCM with different thickness of SiO₂ shell. Simultaneously, the aluminum nanoparticles with different diameters as heat transfer enhancement materials were added into PCM to study the mobility of the nanoparticle-enhanced PCM [19]. Afterwards, the dissipative particle dynamics method was performed to simulate the evolution of the formation process of MEPCM with different constituents [1,20,21].

Our previous molecular dynamics simulations simulated the MEPCM with inorganic shell, which means that the total number of atoms is small and the whole structure is relatively simple. So the whole capsule of appropriate size can be easily constructed and normally simulated. But if the shell of MEPCM is organic, the number of MEPCM atoms will be huge because the shell materials are usually high polymers. Thence, the simulation requires extremely high performance computers and it is extraordinarily time-consuming. Simultaneously, the models of MEPCM are extremely difficult to construct because of multicomponent, the spherical appearance and the boundary condition. However, in order to understand the microscopic mechanisms of heat and mass transfer, the model can be simplified by studying certain specific portion of MEPCM. In this paper, the MEPCM composed of paraffin and polystyrene was taken into consideration and the model was constructed with n-octacosanoic, n-docosane and polystyrene in a cubic cell to investigate the diffusion and thermal conductivity of the mixed part of paraffin and polystyrene by utilizing molecular dynamics method and non-equilibrium molecular dynamics method. This work investigated the microscopic properties, namely diffusion, structural feature and thermal transport, of MEPCM composed of organic shell material and paraffin core by MD and NEMD methods for the first time.

2. Model and method

Fig. 1 displays the structures of n-octacosanoic, n-docosane, polystyrene and their mixture, respectively. In our study, the polystyrene consists of fifteen repeating styrene units with 242 atoms. To construct the amorphous bulk, 15 n-octacosanoic molecules, 15 n-octacosanoic molecules and 5 polystyrene molecules were randomly put together, which has 3520 atoms in all. The system is under periodic boundary condition and possesses cubic lattice geometry. But this initial structure is obviously unreasonable because the molecules may have bad connections and the potential energy of system may not be minimum which can lead to the unstable initial structure. To eliminate the unstable conformations, search for low energy structures and ensure the correctness of subsequent simulations, the anneal simulations were employed to avoid the potential energy of system representing a local minimum. Specifically, five anneal cycles within range from 298 K to 398 K were implemented with a heating ramp of 10 K under micro canonical (NVE) ensemble. The simulated time of anneal treatment sustains 1000 ps. During the anneal simulations, energy (potential energy, kinetic energy, non-bond energy) fluctuates with temperature rising and falling as shown in Fig. 1 (a) and Fig. 2 (b). The potential energy is stored as heat energy. Fluctuation of potential energy means the absorption and release of heat energy. In this process, the molecules continuously adjusted themselves to make the whole system cross energy barrier.

Although anneal operation eliminated unstable or irrational conformations, but the whole process of anneal is actually the process of alternate temperature rising and falling. Therefore, the density of system is always changing and the system is not steady. The isothermal-isobaric (NPT) ensemble was used to equilibrate the system so that a relatively stable density would be obtained. As can be seen from Fig. 2 (c), the cell length of amorphous cell which corresponds to density was constantly changing during the total simulation time of 1000 ps. Ultimately, the density of system fluctuated around 0.9 g cm⁻³, and the length of cubic cell maintained around 32.4 Å. In this process, the energy of system undulated with a small amplitude in Fig. 2 (d).

Consecutively, the temperature rising simulation with an interval of 20 K from 283 K to 463 K was employed to learn the diffusion of the system by observing and analyzing dynamics trajectory, which contributes to understanding microscopic mechanisms of mass transfer of this system.

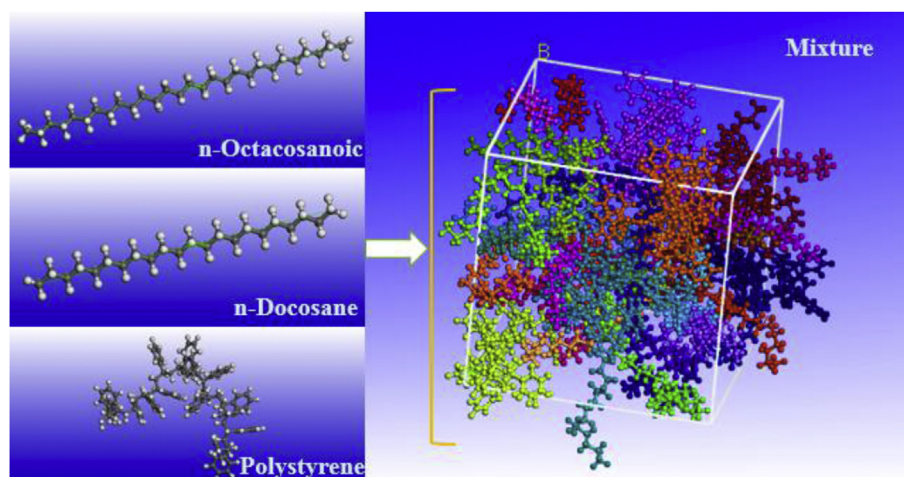


Fig. 1. The structures of n-octacosanoic, n-docosane, polystyrene and their mixture with periodic boundary condition.

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