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Molecular dynamics simulation of thermal physical properties of molten iron

Hong-Jie Yan [a], Jia-Cai Zhuang [a], Ping Zhou [a], Qing Li [a], Chenn Q. Zhou [a,b,*], Pei Fu [a]

[a] School of Energy Science and Engineering, Central South University, Changsha, Hunan 410083, PR China
[b] Central for Innovation through Visualization and Simulation, Purdue University Calumet, 2200 169th Street, Hammond, IN 46323, USA

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ABSTRACT

Physical properties of molten iron at 1500–2500 K, which are poorly understood at high temperature and in undercool state, are calculated based on the molecular dynamics method in this paper. The model of molten iron is developed by LAMMPS. The embedded atom method potential is applied to calculate the interaction between iron atoms. The system is heated to 2500 K, then cooled to the target temperature to obtain the molten iron. Different physical properties of molten iron between 1500 K and 2500 K, including the density, the viscosity, the specific heat capacity and the self-diffusion coefficient, are calculated using the proposed model. The accuracy of the method is validated by comparing the numerical results with the available data in the literature. It is found that almost all the physical properties of molten iron at 1500–2500 K can be accurately calculated with the molecular dynamics method. However, owing to the fact that the specific heat of liquid metal is sensitive to the potential function, the numerical deviation of the specific heat is larger.

1. Introduction

The physical properties of molten iron are of great importance in blast furnace iron making process. In the past several decades, a number of experiments [1–5]and theoretical calculations [6,7] have been carried out to obtain these properties. All of these studies showed that the properties, including the density, the viscosity, the heat capacity, the self-diffusion coefficient and the thermal diffusivity, are affected by temperature. Beutl et al. [1] investigated the specific heat and various dependencies among enthalpy, electrical resistivity, temperature, and density for molten iron up to 5000 K. Wille et al. [5] used a CO_2 laser to heat molten iron and obtain the ratio of the melting enthalpy versus the heat capacity of molten iron. The density of molten iron has been deduced from the image size and the mass of the molten iron drops. Nishi et al. [4] measured the thermal diffusivity of molten iron at temperatures close to 1900 K by a laser flash method. Zhang et al. [6] calculated the diffusion parameters over a broad temperature range and pressure range based on the available P-V-T equation of state of iron. The above research provides abundant data for physical properties of molten iron. Owing to the oxidation of the molten iron, interaction between iron and vessel, and the limited measurement accuracy under high temperature, comprehensive and complete data regarding physical properties are hard to obtain. Specifically, in special conditions, such as high pressure and overcooled states, physical properties are difficult to measure accurately.

With the continual enhancement of computer processing power, the molecular dynamics method has become an important method of calculating the properties of materials, as it is unaffected by the limitations of experimental conditions, such as high temperature and pressure, by calculating in the micro level of system. Physical properties of material, the diffusion process between the various substances, can be calculated under various environmental conditions via the molecular dynamics method. Therefore the molecular dynamics simulation technology has been widely applied in material science, biology, etc. [8–14].

Research on the physical properties of liquid metal using molecular dynamics simulation has been increasingly reported in recent years [15–19]. Yu et al. [15] used the molecular dynamics method to study the transport coefficients and the infinite frequency shear modulus of molten iron at high temperatures and high pressures. The result showed that both shear viscosity and diffusion coefficient along the melting line rise simultaneously, and liquid iron can vitrify under Earth-core conditions. Koci et al. [16] applied the molecular dynamics method to study the properties of molten

* Corresponding author at: Central for Innovation through Visualization and Simulation, Purdue University Calumet, 2200 169th Street, Hammond, IN 46323, USA.
E-mail address: czhou@purduecal.edu (C.Q. Zhou).

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iron under the pressure-temperature conditions of the Earth's outer core. In addition, using the molecular dynamics method, Cao et al. [17] have calculated the transport coefficients under high temperature and Earth-core pressure conditions.

From the current research status, we can see that the molecular dynamics simulation of molten iron research has mainly concentrated on hot metal viscosity and the diffusion coefficient at very high temperatures and pressures, while the physical properties near the melting point and in the overcooled state are rarely examined. In most of metallurgical processes, molten iron temperature is in the range 1800–2500 K. And the thermal physical properties of molten iron have great effect on the quality of iron products. Therefore, the aim of the present work is to study the physical properties of the pure molten iron at 1500–2500 K using the molecular dynamics method.

2. Methodology

Molecular dynamics modeling is a computer simulation of nuclear motion. The structure and properties of the system can be calculated by statistical average method, in which the movement of every atom is based on Newton's second law under the empirical potential field provided by all other atomic nuclei and electrons [20]. This method builds a bridge between purely theoretical studies and experimental research, and all the information in the process of thermodynamics can be output. The temperature and pressure can be freely chosen in the molecular dynamics simulations. Moreover, the method can provide the temperature and the pressure that are difficult to reach within experiments, and the physical properties of the materials can be obtained under extreme conditions.

From the perspective of the potential energy function, it is difficult to use pair potential, three-body potentials to approximate the interaction between metal atoms, because the metal belongs to special material [21]. The embedded atom method (EAM) is usually adopted to simulate the interaction between metal atoms, which can obtain the mechanical and thermodynamic properties of metals [22]. The total potential energy U of the system is expressed by the following equation:

$$U = \sum_i \left[F_i(\rho_i) + \frac{1}{2} \sum_{j(j \neq i)} \phi_{ij}(r_{ij}) \right] \quad (1)$$

where F_i is the embedding function for atom i, ρ_i is the electron density of atom i embedded in the background, and ϕ_{ij} is the pair potential interaction between atom i and j. In addition, r_{ij} is the distance of atom i and atom j.

In this paper, the EAM potential function between iron atoms proposed by Mendelev [23] was adopted. The size of the simulation system was $20 \times 20 \times 20$ $(a_{Fe})^3$. The structure of iron cell was BCC (Body-Centered Cubic) structure, and the lattice constant was a_{Fe} = 2.87 Å. The total number of atoms was 16,000 in this system. The periodic boundary conditions were used in x, y and z directions, and the Nose-Hoover method was used to control the temperature and pressure of the system. The initial velocity distribution of Fe atoms was given according to the Maxwell velocity distribution. The verlet-velocity method was used to integrate the Newton equation numerical integration, in which the time step was 2 fs. The master list distance cutoff in our simulation is 7.3 Å. LAMMPS (large-scale atomic/molecular massively parallel simulator) is a free open-source code which excels at the molecular dynamics of metals. We can calculate the thermal physical properties with suitable potential energy function. The present study used LAMMPS to run the simulation.

In order to obtain high temperature molten iron, the initial model was heated to 2500 K from 1 K and then cooled down to the target temperature. The heating process is shown in Fig. 1. It can be determined from the phase-change curve that the iron is transformed from the solid state to the liquid state when the volume of the system increases sharply. Fig. 1 shows that the iron is still in the solid state when it is heated to 2000 K. The cause of overheating lies in that the initial Fe model is composed of a number of cells, which are perfect crystals with no interface, no defects, and the overall energy is at a minimum level. However, real iron has different degrees of defects, which leads to higher overall energy. Therefore the temperature is usually higher than the actual melting point 1812 K of the iron in molecular dynamics simulations [24]. When heating the iron to a high temperature, and then cooling it to about 1500 K, we find that the iron is still in the liquid state, which is undercool state. Therefore, the iron is heated to 2500 K from 1 K and then gradually cooled down to the target temperature to obtain the molten state of iron at the target temperature, where the heating and cooling rates are 1 K ps^{-1}. Physical properties of molten iron at the target temperature in the subsequent calculation are obtained by this method.

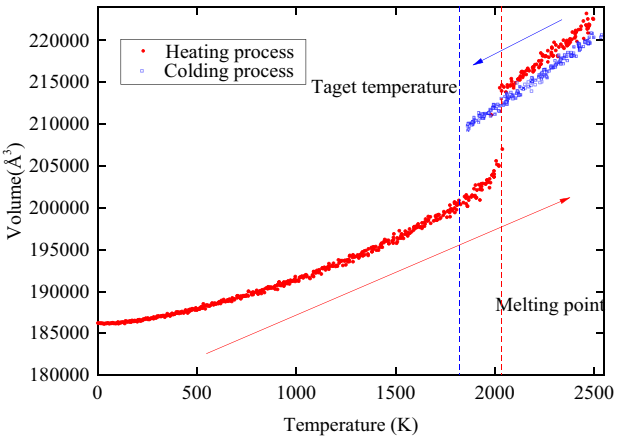

Fig. 1. Heating and cooling process to the target temperature.

3. Results and discussion

3.1. Calculation on density of molten iron at different temperatures

There is abundant experimental data [1,25–32] on the density of molten iron at and above the melting point. However, in the undercool state, few results were reported about the density of

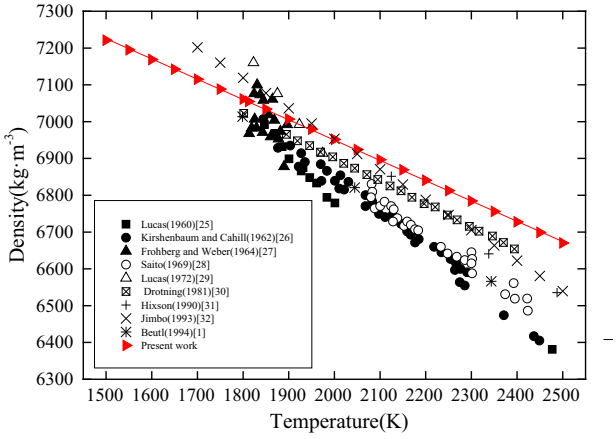

Fig. 2. Density of molten iron at different temperatures.