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Relation of cooling rate, undercooling and structure for rapid solidification of iron melt

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ABSTRACT

It is well known that cooling rate (R_c), undercooling (ΔT) and microstructure in solidification are not independent, but the simple relationships are rarely reported. We aim to present the relation of R_c, ΔT and microstructure through solidification of iron melt by molecular dynamics simulation and classical nucleation theory (CNT). The results show that if $R_c \leqslant 10^{11.97}$ K/s, the iron melt will solidify as bcc crystal structure; if $10^{11.98}$ K/s $\leqslant R_c \leqslant 10^{12.3}$ K/s, the mixed structure of crystalline and glass will be obtained; if $R_c > 10^{12.3}$ K/s, the iron melt will solidify as amorphous structure. From the CNT, a relationship between R_c and ΔT can be deduced, by which, the critical cooling rate for forming glass is predicted as $10^{11.43\pm1}$ K/s that is near the simulation result ($R_c > 10^{11.97}$ K/s).

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1. Introduction

Solidification is a common method for preparation of metallic materials. Researches on solidification of metallic melts are important for the development of phase transformation theories and the improvement of material properties [1,2]. Since the material properties depend on the microstructures [3], in order to enable metallic materials with excellent properties, it is necessary to understand the microstructure evolution upon solidification process. However, in many cases, the transformation process cannot be observed directly, or the experimental required condition cannot be realized by the current techniques, so the computer simulation techniques can make up for the lack of experiment and give an efficient way to display the transformation process [4–15]. With molecular dynamics simulation, Shibuta et al. derived the CCT diagram for nanoparticles by studied the effect of the cooling rate on the solidification behavior of metal nanoparticles, and they found thermally activated homogeneous nucleation can occur spontaneously without any inducing factor [4,5]. With a large-scale molecular dynamics simulation, Hou et al. studied the cooling rate dependence of solidification for liquid aluminum and found the formation mechanism of bulk nanocrystalline aluminum with multiply twinned grains [6,7]. Li et al. studied the structural evolution of TiAl alloy from rapid solidification by the molecular dynamics simulation, and found that at fast cooling rates the amorphous phase can be obtained while at slow cooling rate γ-TiAl + α_2-Ti_3Al [8] phases can be obtained.

Iron is one of the most important raw materials in industry. By measuring liquid structure of pure iron using X-ray diffraction, Waseda et al. found that the crystalline and amorphous structures can be distinguished by the radial distribution function (RDF) [9]. Based on X-ray diffraction experiment, Inui et al. substituted structural parameter into Born-Green equation derived the atom potential of iron [10]. However, both Wareda and Inui's did not observe the solidification of metallic melts visually. In the following years, the developing computer technology made up this lacking. Ganesh et al., using ab initio calculation method, studied the order of short-range structures in undercooled liquid and quantifies icosahedral and polytetrahedral order in supercooled metallic liquid [11]. Pan et al. simulated the formation of groups cluster by molecular dynamics method [12], and found that the radial distribution function of the second peak splitting is because of the irregularity of groups cluster connection. In addition, Cheng et al., using long-range F-S potential simulated the alpha Fe and gamma Fe under different temperatures [13], and found that the first and second peaks in the RDF evolve into a single peak when alpha/gamma phase transition occurs. Liu et al. simulated the high temperature phase transformation by the long-range F-S potential of molecular dynamics method, determined the transition temperature of gamma Fe → delta Fe to be 2132 K and delta Fe → liquid phase to be 2550 K [14]. Shibuta et al. studied the linkage between the empirical interpretation and the atomistic nature in iron, revealed that there exists a critical temperature at which the nucleation rate becomes maximum and the incubation time for the first nucleation

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becomes the shortest by the large-scale molecular dynamics simulation [15]. Nevertheless, all those studies mainly considered the influences of transformation temperature on the structure of Fe, but rarely considered the relation of cooling rate and undercooling.

In this work, the molecular dynamics simulation was used to study the solidification of Fe melt under different cooling rates, and then combining the theoretical calculation, the critical cooling rate for forming glass of Fe melt was determined. Furthermore, the effect of cooling rate on the undercooling for solidification was discussed.

2. Computation details

The solidification of Fe melt was simulated by the software LAMMPS, subjected to 3D periodic boundary conditions and Nose-Hoover Hot bath temperature controlling algorithm with a cubic box including 11,664 atoms (Fe). EAM potential function is from Ref. [16], and the time step is 2 fs.

The simulation of solidification process for Fe melt can be described as: the bcc structure Fe is heated to 2169.6 K and let the system run 50,000 steps to obtain liquid Fe, then held at 2169.6 K for 500,000 steps to obtain the equilibrium liquid; then the system is quenched to 50 K with different cooling rates; then held at 50 K for 500,000 steps; finally, the microstructures were analyzed by RDF, H-A (Honeycutt-Andersen) bond-type index and mirror bonding methods. In the simulation, NPT (isothermal-isobaric) constant is employed, where pressure P and temperature T were imposed by Nose–Hoover method [17].

3. Results and discussions

3.1. RDF analysis

Radial distribution function (RDF), also known as pair distribution function, describes how density varies as a function of distance from a reference atom. RDF $g(r)$ is defined as:

$$\rho g(r) = N^{-1}\left\langle \sum_{i\neq j}\sigma(r+R_i-R_j)\right\rangle \tag{1}$$

where ρ is the average density of system, R the atoms position, bracket ⟨ ⟩ means average by time; σ is the Dirac function; N is the atom number. Considering that RDF has been used to examine the molecular-level structuring for long time [18], it is thus an important function for characterization of the melt and glass structures, even for the short order of the structure. From RDF, many information of a system can be obtained, such as radius of atoms, average atomic spacing and coordination number.

For iron melts subjected to cooling rates of $10^{11.0}$ K/s–$10^{16.0}$ K/s, the corresponding RDF results are shown in Fig. 1. It can be found that, when the cooling rates are $10^{11.0}$ K/s and $10^{11.97}$ K/s, the peaks of RDF curves are sharpened, indicating a main crystalline structure. When the cooling rate is larger than $10^{11.98}$ K/s, with increasing cooling rate, the width of the first peak gradually increases, and the others peaks in the right are gradually weakened and eventually disappear. It suggests that with increase of cooling rate, the percentage of crystalline structure decreases while that of the glass structure increases. When the cooling rate is $10^{12.0}$ K/s, the second peak vanishes and a convex platform appears. When the cooling rate increases to $10^{15.0}$ K/s, the first peak shows as bread curve, which is similar to the RDF curve for liquid structure.

From the discussion above, when the cooling rate is less than $10^{11.97}$ K/s, the melt will solidified as crystalline structure; when the cooling rate is larger than $10^{11.98}$ K/s, it will form as amorphous structure, that is, the critical cooling rate for forming glass structure is $R_c > 10^{11.97}$ K/s.

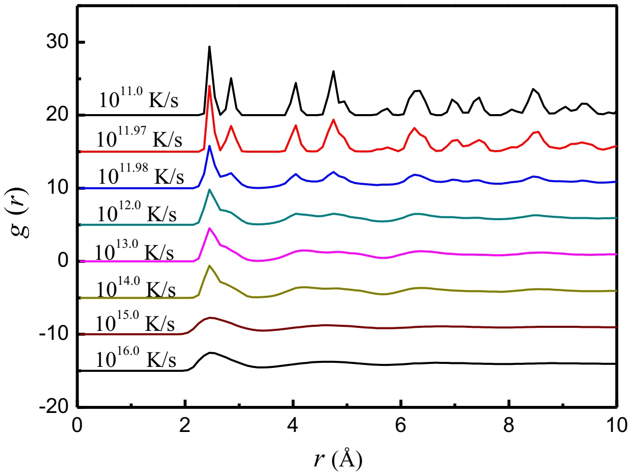

Fig. 1. RDF curves of iron structures from different cooling rates.

3.2. Potential energy curve analysis

From the simulation results, the evolutions of potential with temperature for different cooling rates are shown in Fig. 2. If $R_c \leqslant 10^{11.97}$ K/s, the slope of the curves have two steep jumps, which implies that the solidification structures are crystalline. Fig. 3 shows the initial temperature of solidification as a function of cooling rate, from which, the solidification undercooling increases with cooling rate. We can find that, the lowest initial temperature of solidification is about 881 K (Fig. 2), thereby, the maximal undercooling for forming crystalline phase is about $\Delta T = 1809-881 = 928$ K. If $R_c \geqslant 10^{11.98}$ K/s, the slope of the potential curve (Fig. 2) has no jump, indicating the absence of latent heat release. Therefore, with sufficiently large cooling rates, the crystallization is completely suppressed due to the insufficient relaxation of the atomic structures, resulting in the strongly non-equilibrium metallic glass in the as-solidified materials.

3.3. Bonding relation

The bonding relations between atoms in the system can be described using the bond-type index method of H-A, which can describe the local atomic structure of system [16]. In this method, when the distance of two atoms is smaller than a certain value, the

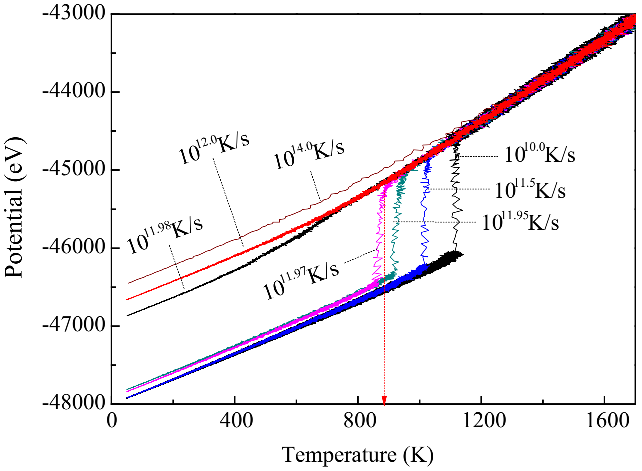

Fig. 2. The temperature dependence of systemic potential energies during cooling at various cooling rates.

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