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Review

Structural and dynamical properties of $Fe_{78}Si_9B_{13}$ alloy during rapid quenching by first principles molecular dynamic simulation

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ABSTRACT

Structural evolution of the $Fe_{78}Si_9B_{13}$ alloy during rapid quenching was investigated by *ab initio* molecular dynamics simulation. The second peak splitting has been perceived even at 1473 K in the partial pair correlation functions though not in the total pair correlation function. The (0, 3, 6, 0) polyhedra are abundant in the liquid state while the distorted (0, 3, 6, 0) polyhedra are the featured local structure around B atoms in the amorphous state. The diffusion coefficients of the three elements are evaluated to understand the dynamics of quenching. From 1173 to 873 K the three coefficients are coherent. We think this temperature range corresponds to the supercooled liquid region, and 873 K serves as the glass transition temperature.

1. Introduction

Fe-based amorphous alloys are important materials which have potential applications. Multi-component amorphous Fe-based steels are paid more attention recently [1,2]. In order to understand the mechanisms of both the formation and crystallization, the knowledge on the structure and its evolution with temperature is important. However, the researchers face intrinsic trouble to investigate the partial structures of multi-component alloys through experimental methods. The classical molecular dynamics simulation is not convenient in most cases to investigate the partial structures due to the lack of proper interatomic potentials. Fortunately, the *ab initio* molecular dynamics simulation (AIMD) provides an easy and efficient way to deal with the partial structural information of the multi-component alloys.

Fe–Si–B alloys are widely studied for many years [3], and are important basic alloys for the development of multi-component magnetic alloys. So it is suitable to employ one of such alloys as a model to study the structural evolution during rapid solidification. Previously we found that in the $Fe_{78}Si_9B_{13}$ alloy the local structure around Si atoms may exhibit rather large difference between the liquid and amorphous structure in the $Fe_{78}Si_9B_{13}$ alloy by AIMD [4]. In this paper, we will present detailed information on the structural evolution of the $Fe_{78}Si_9B_{13}$ alloy with temperature. We can also monitor the change of the diffusion coefficients with temperature. In this way we tried to perceive the supercooled liquid region and glass transition. We hope the results from such a model alloy could strengthen the understanding of the multiple component alloys.

2. Methodology

The AIMD simulations were carried out using the most recent version of the Vienna *ab initio* simulation package (VASP) [5] in which the interactions between the ions and electrons are described by the projector augmented-wave method [6]. Simulations were performed using a gradient corrected energy functional [7]. The plane-wave basis set contained components with energies up to 319.0 eV which is the default value supplied by the pseudopotentials of the VASP package. We also tested a cutoff energy which is 20% larger than the default value at 1473 K; the resulted six independent partial pair correlation

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functions (PCFs), *i.e.* $g_{FeFe}(r)$, $g_{FeSi}(r)$, $g_{FeB}(r)$, $g_{SiSi}(r)$, $g_{BSi}(r)$ and $g_{BB}(r)$ are plotted in Fig. 1. The first peak of $g_{FeFe}(r)$ slightly shifts towards right by 0.0014 nm, the difference in $g_{FeSi}(r)$ and $g_{FeB}(r)$ is hard to determine. In addition, the difference in the other three PDFs is difficult to be distinguished from the statistic error. So, we think that it cannot cause the marked difference to use a larger cutoff energy than the default one. In the following simulations, we then use such default cutoff energy to save computation time.

When dealing with ferromagnetic elements such as Fe, it is rational to take the electronic spin into consideration. Fig. 1 also includes the PDFs with spin effect at 1473 K. In general, the influence of spin on the PDFs is similar to that of enlarging cutoff energy. Among the three PDFs related with Fe element, only the first peak of $g_{FeFe}(r)$ is found to shift slightly towards right by 0.003 nm, the difference in $g_{FeSi}(r)$ and $g_{FeB}(r)$ is also hard to determine. In Ref. [8], the first peak of the pair distribution function of liquid Fe shifted towards right by 0.007 nm after the electronic spin was taken into consideration, and the $g(r)$ looked more ordered than that without spin effect. In the present work, the influence of spin is suppressed by alloying with Si and B elements. In addition, we think it is difficult to attribute the difference in $g_{SiSi}(r)$, $g_{SiB}(r)$ and $g_{BB}(r)$ to the spin effect. On the scale as in Fig. 1 the PDFs with spin are in good agreement with that of no spin effect. If the spin effect is taken into consideration, the computation time will increase many times for the same simulation without spin effect. So, in the following simulations, no spin effect is taken into consideration.

A cubic cell containing 77 atoms (60 Fe atoms, 7 Si atoms and 10 B atoms) with periodic boundary condition was used to simulate the liquid system whose composition is actually 77.9221% Fe, 9.0909% Si and 12.9870% B, very close to the composition of commercial $Fe_{78}Si_9B_{13}$ alloy. We employed the same density 91/nm^3 during the simulations. Generally only the Γ-point was used to sample the supercell Brillouin zone. All the simulations were carried out in the canonical ensemble (NVT) through a Nosé [9] thermostat with a characteristic frequency equals 52 ps^{-1}. Newton's equations of motion were integrated using the Verlet algorithm with a time step of 3 fs. The system was equilibrated at $T = 1473$ K for 9 ps with 2000 configurations from the last 6 ps period being collected for structural analysis. Then the last configuration was quenched at a cooling rate of 3.33×10^{14} K/s towards 300 K. At 1373, 1273, 1173, 1073, 973, 873, 773 K, the configurations were simulated for 6 ps to provide structural information.

3. Results and discussion

3.1. Partial pair correlation functions

Since the $g_{FeFe}(r)$ and $g_{FeSi}(r)$ are rather normal, *i.e.* not rich in structural information, we only present the other four PCFs in this

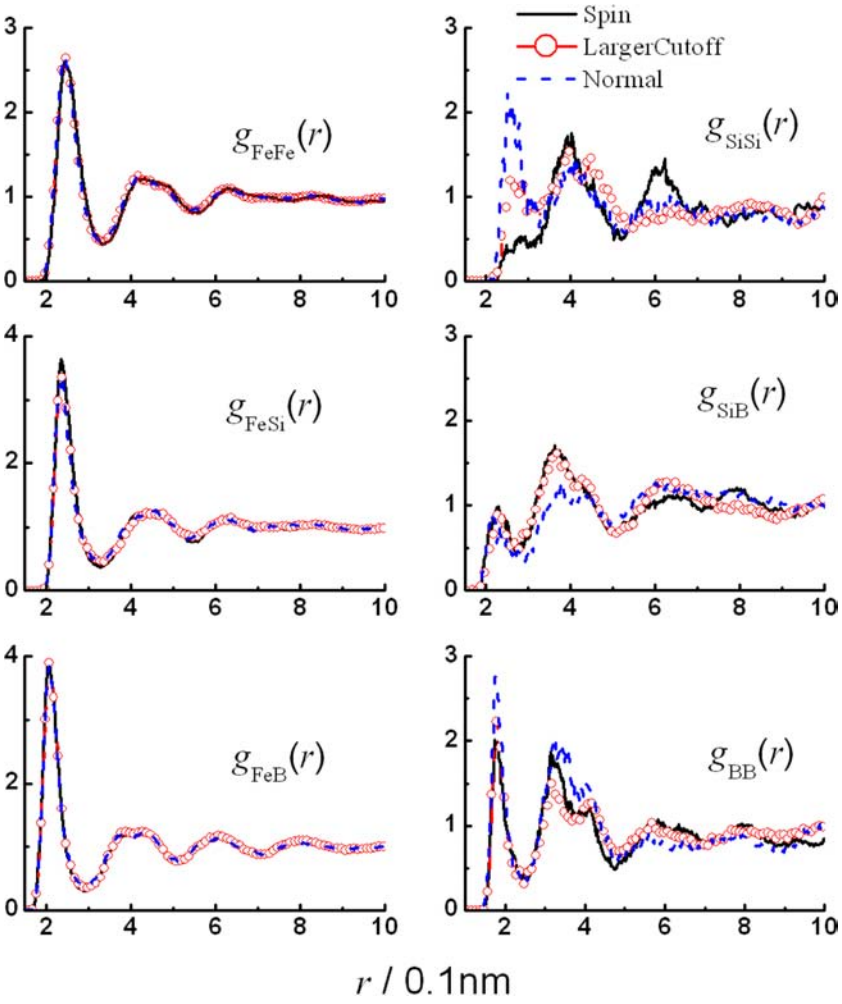

Fig. 1. PDFs of liquid $Fe_{78}Si_9B_{13}$ alloy at 1473 K for three different situations: default cutoff energy (blue dash, labeled as Normal), 1.2 times of the default energy (red line plus open circle, labeled as LargerCutoff), default cutoff energy with spin effect (black line, labeled as Spin). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)