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Evolution of icosahedral clusters during the rapid solidification of liquid TiAl alloy

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ABSTRACT

The evolution characteristics of icosahedral clusters during the rapid solidification of TiAl alloy under different cooling rates are investigated based on molecular dynamics simulations. The short-range order structural properties of liquid and amorphous TiAl alloy are analyzed by several structural characterization methods. It is found that the cooling rate plays a key role during the evolution of icosahedral clusters and has significant effect on the glass transition temperature. Simultaneously, the medium-range order structural evolutions are described in detail by quantitative method and visualization technology during the rapid solidification. The results reveal that the medium-range order icosahedral clusters have good structural stability and configural continuity during the rapid cooling process. Furthermore, the icosahedral structures have significant improvements with decreasing cooling rate. The structures block the crystal nucleation and improve the glass forming ability of supercooled liquid.

1. Introduction

According to years of efforts in experiments and simulations, researchers regard the TiAl alloy as the next-generation high-temperature structural material in the aerospace and automotive fields [1–3]. However, the poor ductility and high chemical reactivity of TiAl-based materials are the main factors limiting the industrial-scale production of TiAl alloy [4–6]. Fortunately, metallic glass (MG) as a newcomer in the world of glass, possesses many excellent properties, such as high yield strength, lower shear modulus, soft magnetic properties, outstanding wear resistance, and superior corrosion resistance [7–10]. It is hoped that the formation of MG will solve these defects in applications of TiAl alloy.

Since microstructure is an accessible signature of stability in MGs, complete structural information is necessary to understand both the atomic arrangement and the formation of clusters. Meanwhile, the icosahedral cluster, as a major structural unit in metallic liquids and glasses, is demonstrated to play an essential role in the glass formation of amorphous alloys [11]. During the rapid solidification, icosahedral clusters in melts not only impact the thermodynamic properties of molten alloys [12,13], but also exhibit excellent structural stability and configural continuity [14,15]. In 1952, Frank [16] first proposed that the icosahedral cluster is the barrier to crystal nucleation in supercooled liquid metals, and this proposal has been verified by numerous scientists in recent years [17,18]. The microstructure of MG strongly depends on the cooling rate during the rapid solidification [19,20]. Until recently, few have reported on the microstructural differences of TiAl alloy which are influenced by different cooling rates. To supplement the shortcomings of this field, computer simulation based on molecular dynamics (MD) is applied as an effective tool which can detect the detailed structural evolutions of the liquid and amorphous TiAl alloy at the atomic level.

In this paper, MD simulation is performed to study the structural and dynamic properties of rapid solidification of TiAl alloy at different cooling rates. The radial distribution function (RDF), bond-angle distribution functions (BAD), Honeycutt–Andersen (HA) bond-type indices, and cluster-type index method (CTIM) are applied to indicate the formations and evolutions of the short-range order (SRO) structures. Moreover, the evolutions of medium-range order (MRO) icosahedral structures during the rapid cooling process are investigated by icosahedral connectivity parameter and visualization technology. The rest of the paper is arranged as follows: the simulation details are presented in Section 2. The results obtained from our simulations are presented and discussed in Section 3. Finally, concluding remarks are given in Section 4.

2. Simulation details

The MD simulations of rapid solidification of liquid TiAl alloy under different cooling rates were carried out using the open

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source code LAMMPS [21]. The system contained 10,976 atoms (5488 Al atoms and 5488 Ti atoms) in a tetragonal box, with this box subjected to the periodic boundary condition. The initial cell arranged as a $L1_0$ structure (a=4.00 Å, c=4.06 Å) [22]. The embedded-atom model (EAM) was developed for the Ti–Al alloys to describe the interatomic interactions in a many-body framework [23]. Simulations were performed in the NPT ensemble with zero pressure and the time step was 1.0 fs. The simulations were started at 2000 K as the melting point of TiAl alloy in experiments is around 1753 K [24]. Firstly, the system was run for 200 ps at 2000 K to guarantee an equilibrium liquid state, and the microstructure was proved to be in a liquid state after this operation. Subsequently, the system was cooled down from 2000 K to 200 K at cooling rates of 10^{13} K/s, 10^{12} K/s, and 10^{11} K/s. During the rapid solidification, atomic positions and other relevant data in the system were recorded with an interval of 100 K. Finally, in order to indicate the SRO and MRO structural evolution of icosahedral clusters which were influenced by different cooling rates, several structural characterization methods were used to analyze the data.

3. Results and discussions

3.1. Radial distribution function

The RDF, the probability of finding a neighboring atom in the spherical shell of a central atom, is widely used to detect the structural characteristics of liquid and glass microstructures. From the $g_{tot}(r)$ curve at 2000 K under cooling rate of 10^{13} K/s in Fig. 1, it can be clearly seen that the formation of TiAl alloy is equilibrium liquid state at the initial temperature [25]. In Fig. 1, the first peak gradually becomes higher and sharper with decreasing temperature, the trough which is between the first and the second peak of the $g_{tot}(r)$ becomes deeper, and a slight split in the second peak of $g_{tot}(r)$ curve can be observed when the liquid is cooled down from 2000 K to 800 K. It is well-known that for many metals, the splitting of the second peak of the $g_{tot}(r)$ curve is the evidence of glass formation and corresponds to the T_g of the system. Therefore, the T_g in this simulation can be considered around 800 K at cooling rate of 10^{13} K/s. The $g_{\alpha\beta}(r)$ curve of partial RDFs as shown in Fig. 2 further reveals that the first peak of $g_{Al-Ti}(r)$ is higher compared with $g_{Ti-Ti}(r)$ and $g_{Al-Al}(r)$. The difference indicates a strong interaction between Al and Ti atoms and some chemical SRO structures indeed exist in the rapidly solidified TiAl alloy. However, it is hard to observe the exact temperature when the secondary peak begins to split according to the $g_{tot}(r)$ curve.

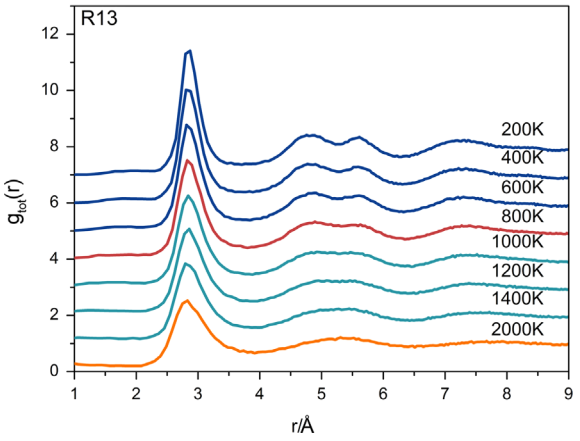

Fig. 1. Evolution of total RDF of TiAl alloy during the rapid solidification under cooling rate of 10^{13} K/s.

The Wendt–Abraham ratio, a further analysis to determine the T_g, is defined as $R=g(r)_{min}/g(r)_{max}$ [26]. The Wendt–Abraham parameter emphasizes the local characteristic of $g_{tot}(r)$, permitting a direct comparison between different structures and leading to a better estimate of T_g [27]. Fig. 3 shows the $g(r)_{min}/g(r)_{max}$ under three different cooling rates 10^{11} K/s, 10^{12} K/s, and 10^{13} K/s. For comparison, the T_g of the TiAl alloy at cooling rate of 10^{11} K/s is depicted in Fig. 3(a), an inflexion of the fitting curve is clearly observed at 700 K, which thus determines the $T_g \approx 700$ K. Similarly, the $T_g \approx 750$ K under cooling rate of 10^{12} K/s is shown in Fig. 3(b), and the $T_g \approx 800$ K under cooling rate of 10^{13} K/s in Fig. 3(c). The calculation of the T_g under different cooling rates reveals the significant effects of cooling rate on the T_g.

3.2. Bond-angle distribution functions

BAD has been calculated for realistic models of MGs and suggests a close analogy of the SRO of topology in the amorphous crystalline states [28]. The curves in Fig. 4 show the evolution of bond angle during the rapid solidification of TiAl alloy under the cooling rate of 10^{11} K/s. It is seen that the curve splits into two peaks centering at approximately 63° and approximately 117° at 2000 K, and the peaks become sharper with decreasing temperature. In addition, a very small and broad peak at approximately 180° is observed around the T_g. We then compared the differences of BAD among the different cooling rates during the rapid cooling process. In Fig. 5, the two peaks at approximately 63° and approximately 117° become sharper with the decrease of cooling rates from 10^{13} K/s to 10^{11} K/s at 200 K.

The ideal coordination pattern of MG is an icosahedron, which features the packing of five slightly distorted icosahedra in the form of a five-fold bi-pyramid, and the ideal icosahedral bond angles are 63.5°, 116.5°, and 180° [28,29]. The results indicate the presence of a large number of icosahedral structures and defective icosahedral structures in MG. Furthermore, TiAl alloy would form more icosahedral structures under the cooling rate of 10^{11} K/s compared with other situations (at cooling rates of 10^{12} K/s, and 10^{13} K/s) during the rapid solidification.

3.3. Sectional analysis

In order to investigate the details of the microstructure in TiAl alloy, we took four sectional drawings at the temperatures of 2000 K, 1400 K, 800 K and 200 K, under the cooling rate of 10^{11} K/s, as shown in Fig. 6. The microstructure of TiAl alloy changed notably during the solidification. Since a small number of triangles were linked by the atoms and bonds at 2000 K, inevitably, plentiful cavities formed between these triangles. At 1400 K, there were still abundant cavities among the liquid phase. When the system cooled down to 800 K (near the T_g), the triangles increased significantly, meanwhile, these triangular structures developed into pentagonal and hexagonal formations. At 200 K, the cavities decreased noticeably, and the volume of these cavities became much smaller. Simultaneously, the pentagonal and hexagonal formations which consisted of triangular structures clearly increased. As the cavities relate to the energy of local structure, a more compact structure forms after the rapid solidification. The ideal icosahedral cluster is packed of five slightly distorted icosahedra in the form of a five-fold bi-pyramid, and the defective icosahedral clusters are formed by five-fold bi-pyramids and six-fold bi-pyramids [28], the result reveals the notable increase of icosahedral structures with the decreasing temperature during the solidification, especially around the T_g.