Computational Materials Science 95 (2014) 502–508

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Glass formation and icosahedral medium-range order in liquid Ti–Al alloys

Zhuo-Cheng Xie [a], Ting-Hong Gao [b], Xiao-Tian Guo [b], Xin-Mao Qin [a], Quan Xie [b,*]

[a] College of Materials and Metallurgy, Guizhou University, Guiyang 550025, China
[b] Institute of New Type Optoelectronic Materials and Technology, College of Electronic Information, Guizhou University, Guiyang 550025, China

ARTICLE INFO

Article history:
Received 7 March 2014
Received in revised form 1 August 2014
Accepted 13 August 2014
Available online 6 September 2014

Keywords:
Ti–Al alloys
Rapid solidification
Icosahedral medium-range order
Glass forming ability

ABSTRACT

In this paper, molecular dynamics simulations are applied to explain the glass formation processes of Ti–Al alloys in structural perspective and to reveal the microstructural evolution of Ti–Al alloys during rapid solidifications in icosahedral medium-range order. The icosahedral medium-range order structural evolutions are described in detail by icosahedral connectivity parameter and coordination number during the rapid solidifications. The results reveal that the icosahedral medium-range order is an appropriate structural unit, which aptly describes glass formation processes of liquid and amorphous Ti–Al alloys in structural aspect. Furthermore, hexagonal connected icosahedral clusters, which link via volume-sharing, have good structural stability and configural continuity, and act as the junction closely connects nearby extended icosahedral clusters. At the same time, the number of the hexagonal formation after the rapid solidification could properly reflect the glass forming abilities of the Ti–Al alloys with different compositions.

1. Introduction

Icosahedral structure, as a major structural unit in metallic liquids and glasses, is demonstrated to play essential roles in glass formations of amorphous alloys and microstructural evolutions of metallic glasses (MGs) [1,2]. From the early discoveries of MGs, most researches focused on the quantitative criterions to indicate the glass forming abilities (GFA) in thermodynamic aspect [3–5]. In this paper, glass formation process of liquid alloy is correlated with microstructural evolution of icosahedral structure during rapid solidification to provide more intuitive information. In 1952, Frank [6] proposed that the icosahedral short-range order (ISRO) structure is the barrier to crystal nucleation in supercooled liquid metals, and this proposal has been verified by researchers [7,8]. With the development of structural investigation, researchers realized that the ISRO structural unit did not presuppose spatial distributions and linking patterns to be some other important structural parameters affecting the structural stability in MGs, so it could not describe the structures beyond the nearest-neighbor atomic shell [9]. The defects naturally lead to the introduction of icosahedral medium-range order (IMRO), the next highest level of structural organization beyond ISRO. The concept of IMRO in amorphous structure was proposed on the basis of structural and thermodynamic considerations [2,10–14]. Among the IMRO structures, the interpenetrating connection of icosahedra (ICOI) is more stable than other types of connected icosahedral clusters [9,15,16]. The growth of the ICOI is considered to be the most important evolution in IMRO structures, which enhances the GFA and mechanical properties of amorphous alloys during rapid solidification [9,15,16].

In recent years, Ti–Al alloys are applied in aerospace and automotive fields as excellent engineering materials due to their high specific strength and stiffness, high strength retention and high creep resistance at high temperature [17–19]. However, the poor ductility and high chemical reactivity of TiAl-based materials are the main factors limiting the industrial-scale production [20–22]. MG has many unique properties that are unusual for metallic crystal, and it provides important new opportunities to improve the material performances of Ti–Al alloys [23–27]. In 1998, Shimono and Onodera [28] first investigated the crystallization and glass formation of Ti–Al alloys under rapid solidification conditions through MD simulation. In 2004, Pei et al. [29] simulated the crystal formation of Ti_3Al alloy under different cooling rates. After that, he further studied the crystallization of liquid Ti_3Al alloy during isothermal annealing [30]. Until now, the IMRO structural evolutions during glass formation processes in Ti–Al alloys have not been established. In this study, computer simulation based on molecular dynamics (MD) is applied as an effective tool to detect the icosahedral evolutions of liquid and amorphous Ti–Al alloys at the atomic level. The glass formation processes of Ti–Al alloys

* Corresponding author. Tel./fax: +86 851 3623 248.
E-mail address: qxie@gzu.edu.cn (Q. Xie).

http://dx.doi.org/10.1016/j.commatsci.2014.08.023
0927-0256/

are indicated through structural characterization methods. The radial distribution function (RDF) is applied to indicate the formation of MG. The cluster-type index method (CTIM) is adopted to indicate the formations and evolutions of the short-range order structures [31]. The evolutions of the IMRO structures are investigated by icosahedral connectivity parameters (C_{ico}) and average coordination number (CN) of center atom of icosahedral cluster. Moreover, we further investigate the evolutions of hexagonal connected icosahedral clusters which connect via volume-sharing in MG during the cooling processes. 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

In this study, we selected eight model alloys from the Ti–Al binary systems: Ti_7Al, Ti_3Al, Ti_5Al_3, TiAl, Ti_3Al_5, $TiAl_3$, $TiAl_7$, and $TiAl_{19}$. The rapid solidifications of liquid Ti–Al alloys were carried out by MD technique. The systems containing 32,000 atoms corresponding to the Ti_7Al, Ti_3Al, Ti_5Al_3, TiAl, Ti_3Al_5, $TiAl_3$, $TiAl_7$, and $TiAl_{19}$ compositions were first packed into cubic boxes (side lengths = 7.9 nm) and subjected to the periodic boundary condition. The simulations employed the embedded-atom model (EAM) which was developed for the Ti–Al alloys to indicate the interatomic interactions in a many-body framework [33]. The simulations were performed in the NPT ensemble with zero pressure and the time step was 1.0 fs. Since the melting points of Ti_7Al, Ti_3Al, Ti_5Al_3, TiAl, Ti_3Al_5, $TiAl_3$, $TiAl_7$, and $TiAl_{19}$ alloys are all below 2000 K [18], the simulations were started at 2000 K. Firstly, the systems were run for 200 ps at 2000 K to guarantee equilibrium liquid states. Since the mean-square displacements of the atoms in these Ti–Al alloys at this temperature from our calculation in 10 ps are larger than the square of the bond length (about 4 Å) in the system, this simulation temperature should be high enough for these liquids to reach thermal equilibrium. Subsequently, the systems were cooled down from 2000 K to 200 K under cooling rate of 10^{11} K/s. The atomic positions in the systems were recorded with an interval of 10 K during the rapid quenching processes. Finally, several structural characterization methods were applied to describe the IMRO structural evolutions of the Ti–Al alloys.

3. Results and discussions

3.1. Glass formations of Ti–Al alloys

In order to investigate the formations of MGs in the Ti–Al alloys, RDF was applied to describe the probability of finding a neighboring atom in the spherical shell of a central atom. In Fig. 1(d–f), notable splits in the second peaks of the $g(r)$ curves can be observed at 800 K, and the notable splits are detected at 500 K as shown in Fig. 1(g and h). Since the split of the second peak in the $g(r)$ curve is the evidence of glass formation, TiAl, Ti_3Al_5, $TiAl_3$, $TiAl_7$, and $TiAl_{19}$ alloys formed amorphous structures during the rapid solidifications at cooling rate of 10^{11} K/s.

As shown in Fig. 1(a–c), the evolutions of RDFs reveals that liquid Ti_7Al, Ti_3Al, and Ti_5Al_3 alloys formed crystalline states during the rapid solidifications at cooling rate of 10^{11} K/s. To further analyze the formation of crystalline structures in the Ti–Al alloys, we took four snapshots of the simulation box with structural type

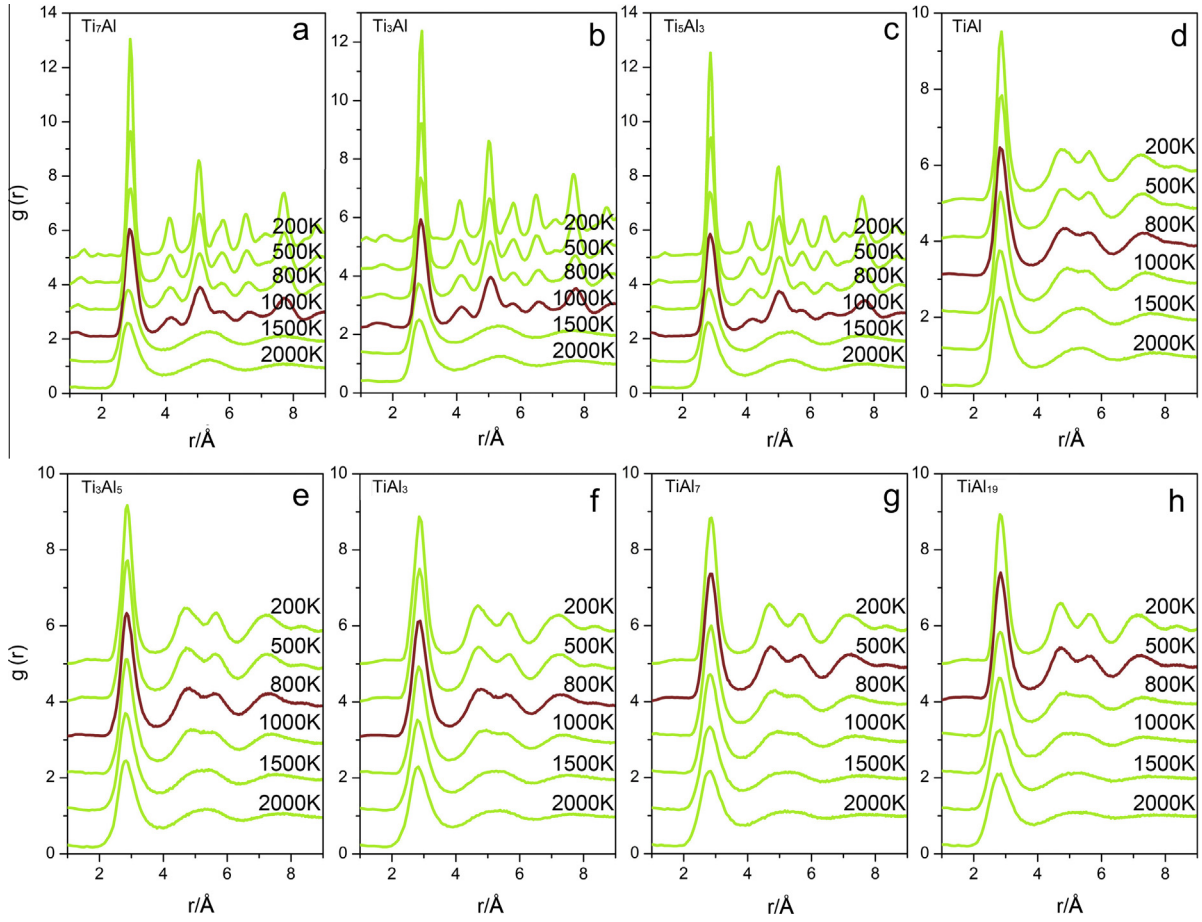

Fig. 1. Evolutions of RDFs of Ti–Al alloys during the rapid solidifications under cooling rate of 10^{11} K/s.