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Liquid state property, structural evolution and mechanical behavior of Ti—Fe alloy solidified under electrostatic levitation condition

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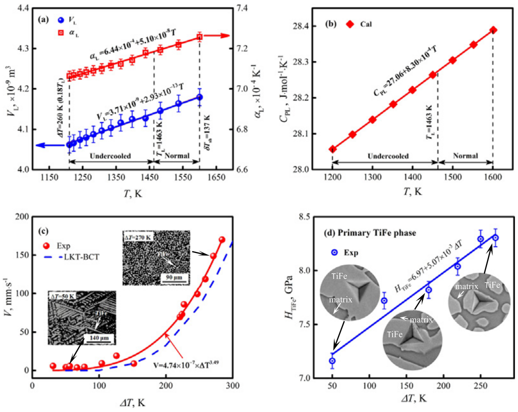
HIGHLIGHTS

- $Ti_{63.64}Fe_{36.36}$ alloy was undercooled up to $\Delta T = 270$ K ($0.18T_L$) by ESL.
- Thermophysical properties for undercooled liquid were measured and calculated by MD.
- Growth velocity of primary TiFe intermetallic compound rises with ΔT up to 170 mm/s.
- Hardness of TiFe increases with ΔT and relates to grain size by Hall-Petch function.

GRAPHICAL ABSTRACT



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ABSTRACT

The thermophysical properties of hypereutectic $Ti_{63.64}Fe_{36.36}$ alloy at both normal and undercooled states, including density, volume expansion coefficient, ratio of specific heat to emissivity were measured by electrostatic levitation (ESL) method combined with a high-speed photography technique. The enthalpy, specific heat, solute diffusion coefficient and surface tension were simultaneously calculated as functions of temperature by molecular dynamics simulation (MD), from which the emissivity was also derived. The rapid solidification kinetics in the undercooling range from 50 K to a maximum value of 270 K ($0.18T_L$) during ESL experiments was quantitatively studied. As undercooling increases, primary TiFe intermetallic compound evolves from coarse dendrites to refined equiaxed grains, whose volume fraction rises significantly. The growth velocity of primary TiFe phase increases according to a power relation with undercooling to a maximum of 170 mm/s, which agrees well with the calculated results from LKT/BCT model on the basis of above determined thermophysical properties. The inter-correlations among "undercooling-microstructure-hardness" were derived subsequently through experiments. The hardness of both primary TiFe intermetallic compound and $Ti_{63.64}Fe_{36.36}$ alloy increases almost linearly with the increase of undercooling, and the former one relates to its grain size by Hall-Petch function.

1. Introduction

Compared with other structural metallic alloys, Ti-based alloys possess many excellent properties, such as light density [1,2], high specific strength [3], low elastic modulus [4], small thermal conductivity

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coefficient [5], extraordinary corrosion resistance [6], and serving under extremely high and low temperatures [7–9], which make them widely applied in the fields of aerospace and industry. From a fabrication point of view, many techniques are utilized to prepare Ti-based alloys, such as powder metallurgy [10], friction stir processing (FSP) [11],centrifugal casting [12], directional solidification [13] and so on, among which the rapid solidification method [14–16] has aroused great interests. There are published reports [17,18] on the rapid solidification mechanism for Ti-based alloys and its relationship with the microstructure evolution in recent years. For example, it was shown that the final solidification morphology of ternary Ti-12Al-8 V alloy depended upon the coupled influences of both liquid undercooling and cooling rate [19].

In fact, the thermophysical properties for undercooled liquid Ti-based alloys, such as density, specific heat, surface tension and diffusion coefficient are indispensable for theoretically describing their rapid solidification kinetics and microstructure evolution [20,21]. However, the relatively high liquidus temperature, the easy oxidization and the high chemical activity of Ti-based alloys are the barriers in achieving their deeply undercooled state, not to mention measuring their metastable thermophysical properties. In such a case, researchers always roughly estimate the thermophysical parameters by Neumann-Kopp's rule (N—K) from the value of each pure component at their melting points, which brings in large discrepancy and leads to the far deviation between theoretical/numerical solidification modeling results and the experimental ones. In addition, computer simulation, such as molecular dynamic (MD) simulation [22,23] and first principles calculation [24] can be used to predict thermophysical properties of liquid alloys versus temperature. However, the validity of simulation results still needs to be confirmed by accurate experimental determination. Fortunately, containerless processing technologies, such as electrostatic levitation (ESL) has been developed and become a powerful tool to overcome this issue. During ESL experiments, the high vacuum environment effectively prevents the oxidation of Ti-based alloys while the containerless state eliminates their chemical reaction with the crucible. As a result, Ti-based alloy melts can be undercooled to a large extent as compared with conventional technology, which makes it possible to measure thermophysical properties versus undercooling before their rapid solidification process achieved. Consequently, the precise thermophysical parameters at varied temperature can be acquired for theoretical analysis on rapid solidification.

As for the mechanical property of Ti-based alloys, it mainly depends on the microstructural evolution during solidification. In general, the increase in undercooling may lead to the variation of phase selection and microstructure transition in rapidly solidified Ti-based alloys, which could tune their mechanical property. Some investigations [25,26] showed that the mechanical properties of Ti-based alloys can be enhanced if they solidify at high undercoolings. Nevertheless, systematic research on the quantitative correlation between undercooling and mechanical property is still on the way.

In present work, by using the ESL technique, binary $Ti_{63.64}Fe_{36.36}$ alloy was deeply undercooled and its rapid solidification was realized. Firstly, the thermophysical properties of the metastable liquid alloy were systematically measured as functions of temperature. Meanwhile, the MD simulation was applied as an assistant to provide supplementary thermophysical information. Secondly, the growth morphology and kinetics of the main primary TiFe internmetallic compound were explored. Finally, the relationship among "undercooling-microstructure-microhardness" was developed as an example to reveal the effect of rapid solidification on mechanical property of binary Ti-based alloys.

2. Experimental procedure and numerical simulation

2.1. Electrostatic levitation processing

The $Ti_{63.64}Fe_{36.36}$ master alloy, whose location was marked in the binary Ti—Fe alloy phase diagram shown in Fig. 1(a), was prepared from 99.999% pure Ti and 99.99% pure Fe elements by arc melting under the protection of Ar atmosphere. The alloy sample was divided into several small portions and remelted by laser to form spherical samples with diameter of 2–3 mm. During electrostatic levitation (ESL) experiments, a spherical alloy sample was initially levitated in a high vacuum environment within an electrostatic field, then was heated to superheated liquid state by SPI SP300 fiber laser with 1070 nm wavelength, and finally solidified by natural cooling. The temperature of the alloy sample was monitored simultaneously by a CellaTemp PA 40 single-color pyrometer with an absolutely accuracy of ±5 K. The expansion coefficient, density and ratio of specific heat to emissivity of the levitated alloy samples were measured by detecting their shape evolution by using the high-resolution CCD camera coupled with a telescopic lens, which was calibrated by levitating a standard steel ball under identical conditions. The dendritic growth velocity of primary TiFe phase under different undercoolings was measured by a Thorlabs PDA 100A high sensitive photodiode (PD).

After experiments, the solidified alloy samples were polished according to the standard metallographic procedure and were etched using a solution of $HF + HNO_3 + HCl + H_2O$ with the volume ratio 1:2.5:1.5:95. The phase constitution of the solidified samples was checked by a Rigaku D/max 2500 X-ray diffractometer (XRD). The microstructures were analyzed by an optical microscope (OM).

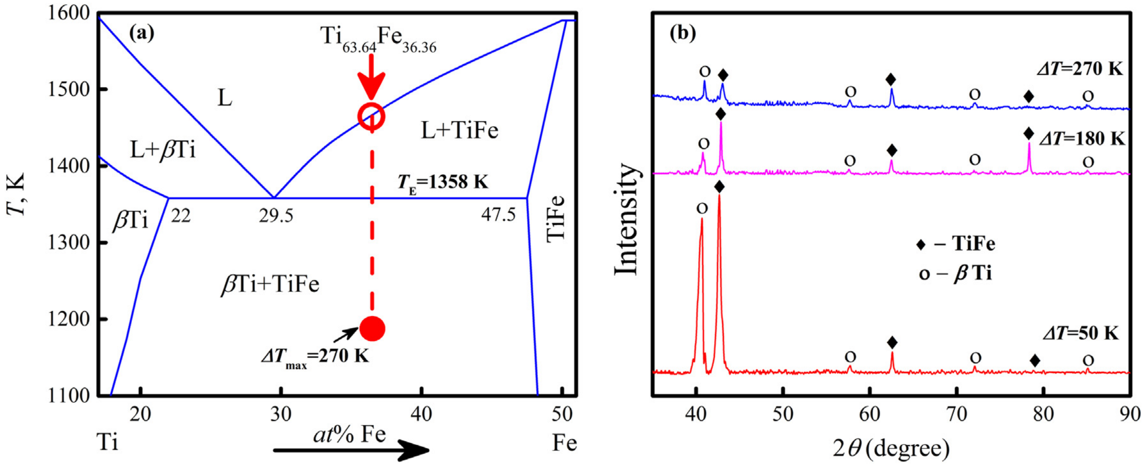

Fig. 1. The composition selection and XRD patterns of $Ti_{63.64}Fe_{36.36}$ alloy: (a) location in phase diagram; (b) X-ray diffraction patterns.