Data and analyses of phase relations in the Ce-Fe-Sb ternary system

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Abstract

These data and analyses support the research article “Experimental study on phase relations in the Ce-Fe-Sb ternary system” Zhu et al. (2017) [1]. The data and analyses presented here include the experimental results of XRD, SEM and EPMA for the determination of the whole liquidus projection and the isothermal section at 823 K in the Ce-Fe-Sb system. All the results enable the understanding of the constituent phases and the solidification processes of the as-cast alloys as well as the phase relations and the equilibrium regions at 823 K in the Ce-Fe-Sb ternary system over the entire composition.

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Specifications Table

| Subject area       | Materials Sciences |
|--------------------|--------------------|
| More specific subject area | Phase diagram and relations |
| Type of data       | Tables, figures, images (x-ray, microscopy, etc.), |

DOI of original article: https://doi.org/10.1016/j.jallcom.2017.09.276
How data was acquired: Microscope, SEM, XRD, EPMA of as-cast and annealed samples

Data format: Raw, analyzed

Experimental factors:

The as-cast samples were prepared and the isothermal heat treatment was conducted as reported in a previous study [1].

Experimental features:

The as-cast alloys were used to determine the primarily crystallized phases, to construct the liquidus projection diagram, and to analyze the solidification processes. And the heat-treated samples were prepared to measure the phase equilibria and to construct the isothermal section.

Data source location:

Data was collected in the School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China. (39°26N, 117°30E)

Data accessibility:

The data are available with this article and within the Ref.[1]

Related research article:

Experimental study on phase relations in the Ce-Fe-Sb ternary system (in press)

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Value of the Data

1. Data

These raw data, containing the experimental results of XRD, SEM and EPMA for the determination of the whole liquidus projection and the isothermal section at 823 K in the Ce-Fe-Sb system, are obtained from Ref. [1].

2. Experimental design, materials, and methods

All experimental design, materials and methods were based on reported paper [1].

2.1. Liquidus projection over the entire composition range

For the liquidus projection of the Ce-Fe-Sb ternary system constructed in present work, there exist 17 primary solidification regions. Except the descriptions of the primary solidification regions (CeSb), (FeSb), \( \tau_1 \), \( \tau_2 \) and \( \tau_3 \) in Ref. [1], the remaining regions are fully shown and described as follows.

Using BSE/BEI images, it should be noted that within the XRD spectra of the as-cast alloys #1–10, some diffraction peaks of CeO2 exist since the very easy oxidation of these Ce-rich alloys after their exposing to air, resulting in the dark-grey distributions of cracks and pits along with the dark phase (\( \gamma \)Ce) within the backscattered electron images.

2.1.1. Primary solidification region of (\( \alpha/\delta \)Fe)

1) Ce-72Fe-25Sb (#1)

The X-ray diffractogram and BEI micrographs of Ce-72Fe-25Sb (#1) as-cast alloy are shown in Fig. 1. The microstructure consists of a large and black primary phase (\( \alpha/\delta \)Fe), a dark+grey two-phase
Fig. 1. Experimental results of Ce-72Fe-25Sb (Å1) as-cast alloy: (a) X-ray diffractogram; (b) and (c) BEI micrographs at low and high magnifications, respectively.
# Table 1
The compositions of the constituent phases existing in the different Ce-Fe-Sb ternary as-cast alloys.

| Phases      | Compositions (at%) | Remarks                  |
|-------------|--------------------|--------------------------|
|             | Ce     | Fe    | Sb    |                     |
| (α/δFe)     | 0.03   | 96.97 | 3.00  | In as-cast #1 alloy |
|             | 0.07   | 98.35 | 1.58  | In as-cast #2 alloy |
|             | 0.16   | 96.24 | 3.60  | In as-cast #11 alloy|
|             | 0.98   | 96.33 | 2.69  | In as-cast #12 alloy|
|             | 0.00   | 95.65 | 4.35  | In as-cast #24 alloy|
|             | 0.11   | 96.18 | 3.71  | In as-cast #25 alloy|
|             | 0.13   | 95.98 | 3.89  | In as-cast #26 alloy|
| (γFe)       | 0.39   | 98.14 | 1.47  | In as-cast #3 alloy |
| Ce₂Fe₁₇     | 12.99  | 87.01 | 0.00  | In as-cast #3 alloy |
|             | 9.55   | 90.45 | 0.00  | In as-cast #4 alloy |
|             | 10.19  | 89.81 | 0.00  | In as-cast #5 alloy |
|             | 10.89  | 89.11 | 0.00  | In as-cast #9 alloy |
|             | 9.59   | 90.41 | 0.00  | In as-cast #10 alloy|
|             | 11.49  | 88.51 | 0.00  | In as-cast #25 alloy|
|             | 10.57  | 89.43 | 0.00  | In as-cast #26 alloy|
| CeFe₂       | 32.99  | 67.01 | 0.00  | In as-cast #3 alloy |
|             | 32.20  | 67.80 | 0.00  | In as-cast #4 alloy |
|             | 32.32  | 67.68 | 0.00  | In as-cast #5 alloy |
|             | 66.08  | 33.92 | 0.00  | In as-cast #6 alloy |
|             | 33.66  | 66.34 | 0.00  | In as-cast #7 alloy |
|             | 33.44  | 66.51 | 0.00  | In as-cast #8 alloy |
| (γCe)       | 98.41  | 0.00  | 1.59  | In as-cast #6 alloy |
|             | 98.60  | 0.00  | 1.40  | In as-cast #7 alloy |
|             | 96.68  | 2.25  | 1.07  | In as-cast #8 alloy |
| (δCe)       | 97.90  | 0.75  | 1.35  | Derived             |
| Ce₂Sb       | 66.92  | 0.00  | 33.08 | In as-cast #3 alloy |
|             | 66.94  | 0.00  | 33.16 | In as-cast #4 alloy |
|             | 67.89  | 0.00  | 32.10 | In as-cast #5 alloy |
|             | 66.94  | 0.00  | 33.06 | In as-cast #6 alloy |
|             | 66.78  | 0.00  | 33.22 | In as-cast #7 alloy |
|             | 66.65  | 0.00  | 33.95 | In as-cast #8 alloy |
|             | 66.70  | 0.00  | 33.30 | In as-cast #9 alloy |
|             | 66.79  | 0.00  | 33.21 | In as-cast #10 alloy|
| Ce₄Sb₃      | 55.90  | 0.00  | 44.10 | In as-cast #9 alloy |
|             | 54.44  | 0.00  | 45.56 | In as-cast #10 alloy|
| (CeSb)      | 49.36  | 0.00  | 50.64 | In as-cast #11 alloy|
|             | 49.68  | 1.11  | 49.21 | In as-cast #12 alloy|
|             | 49.66  | 0.00  | 50.34 | In as-cast #13 alloy|
|             | 49.47  | 0.00  | 50.52 | In as-cast #14 alloy|
|             | 49.82  | 0.10  | 50.07 | In as-cast #15 alloy|
|             | 48.73  | 0.75  | 50.52 | In as-cast #16 alloy|
|             | 48.50  | 1.61  | 49.88 | In as-cast #17 alloy|
|             | 48.71  | 1.61  | 49.68 | In as-cast #25 alloy|
|             | 48.62  | 1.59  | 49.79 | In as-cast #26 alloy|
| βCeSb₂      | 33.42  | 0.12  | 66.46 | Derived             |
| αCeSb₂      | 33.96  | 0.00  | 66.04 | In as-cast #18 alloy|
|             | 33.16  | 0.00  | 66.84 | In as-cast #19 alloy|
|             | 33.50  | 0.69  | 66.50 | In as-cast #20 alloy|
|             | 33.94  | 0.00  | 66.06 | In as-cast #21 alloy|
|             | 33.03  | 0.00  | 66.97 | In as-cast #22 alloy|
eutectic (α/δFe)+(FeSb) divorced to some degree, and a grey + white two-phase eutectic (FeSb)+τ3 which was also divorced. The crystal structure and the composition of the different phases were determined using XRD and EPMA respectively. Within the XRD spectra of the as-cast samples as shown in Fig. 1(a), some diffraction picks of Ce2O3 exist since the very easy oxidation of the Ce-containing alloys after their exposing to air. The average compositions of the primary solidification phase (α/δFe) and the subsequent solidification phases (FeSb) and τ3 in the divorced eutectic structures are Ce-96.97Fe-3.00Sb, Ce-54.21Fe-44.00Sb and Ce-36.86Fe-44.97Sb respectively as listed in Table 1.

2) Ce-60Fe-33Sb (#2)

The microstructure of Ce-60Fe-33Sb (#2) as-cast alloy consists of a large and grey primary phase (α/δFe) with an average composition of Ce-98.35Fe-1.58Sb and an almost equal amount of white τ3 phase of Ce-35.89Fe-46.88Sb resulting in a divorced two-phase eutectic (α/δFe)+τ3 (Fig. 2).
Fig. 2. Experimental results of Ce-60Fe-33Sb (#2) as-cast alloy: (a) X-ray diffractogram; (b) and (c) BEI micrographs at low and high magnifications, respectively.
Fig. 3. Experimental results of Ce-58Fe-2Sb (#3) as-cast alloy: (a) X-ray diffractogram; (b) and (c) BEI micrographs at low and high magnifications, respectively.
Fig. 4. Experimental results of Ce-51Fe-2Sb (#4) and Ce-42Fe-6Sb (#5) as-cast alloys: (a) X-ray diffractogram of #4 alloy; (b) and (c) BEI micrographs of #4 and #5 alloys, respectively.
2.1.2. Primary solidification region of (γFe)

Ce-58Fe-2Sb (#3)

The microstructure of Ce-58Fe-2Sb (#3) as-cast alloy consists of a small and black primary phase (γFe), a dark-grey phase Ce₂Fe₁₇ which grew in a peritectic-type manner from the phase (γFe), a light-grey phase CeFe₂ and a light-grey + white two-phase eutectic CeFe₂ + Ce₂Sb. The primary phase (γFe) is of a small volume fraction, indicating that the nominal composition of #3 as-cast alloy is very close to the peritectic ridge L₁ + (γFe) → Ce₂Fe₁₇ (Fig.3).

2.1.3. Primary solidification region of Ce₂Fe₁₇

Ce-51Fe-2Sb (#4) and Ce-42Fe-6Sb (#5)

The microstructures of Ce-51Fe-2Sb (#4) and Ce-42Fe-6Sb (#5) as-cast alloys consist of a dark flaky primary phase Ce₂Fe₁₇, a grey phase CeFe₂ which grew in a peritectic manner from the phase Ce₂Fe₁₇, and a grey + white two-phase eutectic CeFe₂ + Ce₂Sb (Fig.4).

2.1.4. Primary solidification region of Ce₂Sb

1) Ce-10Fe-10Sb (#6)

The microstructure of Ce-10Fe-10Sb (#6) as-cast alloy consists of a large and white dendrite primary phase Ce₂Sb, a white + dark two-phase eutectic Ce₂Sb + (γCe) and a white + dark + grey three-phase eutectic Ce₂Sb + (γCe) + CeFe₂ (Fig. 5).
Fig. 7. Experimental results of Ce-10Fe-20Sb (#9) and Ce-22Fe-16Sb (#10) as-cast alloys: (a) X-ray diffractogram of #9 alloy; (b) and (c) BEI micrographs of #9 and #10 alloys, respectively.
2) Ce-22Fe-8Sb (#7) and Ce-30Fe-10Sb (#8)

Ce-22Fe-8Sb (#7) and Ce-30Fe-10Sb (#8) have the similar as-cast microstructure as shown in Fig. A6, consisting of a large and white dendrite primary phase Ce₂Sb, a white + grey two-phase divorced eutectic Ce₂Sb + CeFe₂ and a white + grey + dark three-phases eutectic Ce₂Sb + CeFe₂ + (γCe) which was also divorced (Fig. 6).

Fig. 8. Experimental results of Ce-8Fe-82Sb (#18) as-cast alloy: (a) X-ray diffractogram; (b) BEI micrograph.

Fig. 9. Isothermal experimental results of Ce-51Fe-2Sb (#4) and Ce-42Fe-6Sb (#5) heat-treated alloys: (a) X-ray diffractogram of #5 alloy; (b) and (c) BEI micrographs of #5 and #4 alloys, respectively.
2.1.5. Primary solidification region of Ce$_4$Sb$_3$

Ce-10Fe-20Sb (#9) and Ce-22Fe-16Sb (#10) as-cast alloys consists of a large dark grey primary phase Ce$_4$Sb$_3$ with an average composition of Ce-44.10Sb, a light grey Ce$_2$Sb phase growing in a peritectic-type manner, and a dark Ce$_2$Fe$_{17}$ phase of Ce-90.41Fe divorced from the two-phase eutectic Ce$_2$Sb + Ce$_2$Fe$_{17}$ (Fig. 7).
2.1.6. Primary solidification region of CeSb₂

Ce-8Fe-82Sb (#18)

The microstructure Ce-8Fe-82Sb (#18) as-cast alloy consists of a white strip primary phase $\alpha$CeSb₂, a white + dark two-phase eutectic $\alpha$CeSb₂ + $\tau_1$ and a large volume fraction of a grey phase (Sb) which is divorced from the three-phase eutectic $\alpha$CeSb₂ + $\tau_1$ + (Sb) since (Sb) is the dominant phase near the Sb corner (Fig. 8).
2.2. Isothermal section at 823 K over the entire composition range

For the isothermal section at 823 K of the Ce-Fe-Sb ternary system constructed in present work, there exist 15 three-phase regions. In Ref. [1], the detailed descriptions of the three-phase regions containing $\tau_2$ phase $(\text{CeSb}) + \tau_2 + \tau_3$, $(\text{CeSb}) + \tau_2 + \alpha\text{CeSb}_2$, $(\text{FeSb}) + \tau_3 + \tau_2$, $\alpha\text{CeSb}_2 + \tau_1 + \tau_2$ and
(FeSb) + τ1 + τ2, are presented. The remaining regions are fully shown in Figs. 9-18 and described as follows. The equilibrium phase compositions of constituent phases in the heat-treated alloys mentioned below are summarized in Table 6 as presented in Ref. [1].

It should be pointed out that within the XRD spectra of some alloys, the diffraction peaks of Ce2O3, Sb2O5 and Fe2O3 exist since the very easy oxidation of these alloys after their exposing to air, resulting in the dark-grey distributions of cracks and pits.
B1 \((\gamma\text{Ce}) + \text{CeFe}_2 + \text{Ce}_2\text{Sb}\) three-phase region \(\text{Ce-51Fe-2Sb}\) (#4) and \(\text{Ce-42Fe-6Sb}\) (#5)
B2 \(\text{Ce}_2\text{Sb} + \text{CeFe}_2 + \text{Ce}_2\text{Fe}_{17}\) three-phase region \(\text{Ce-60Fe-10Sb}\) (#27) and \(\text{Ce-71Fe-3Sb}\) (#28)
B3 \(\text{Ce}_2\text{Sb} + \text{Ce}_4\text{Sb}_3 + \text{Ce}_2\text{Fe}_{17}\) three-phase region \(\text{Ce-10Fe-35Sb}\) (#29)
B4 \((\text{CeSb}) + \text{Ce}_2\text{Fe}_{17} + (\alpha\text{Fe})\) three-phase region \(\text{Ce-51Fe-23Sb}\) (#30)
B5 \((\text{CeSb}) + \tau_3 + (\alpha\text{Fe})\) three-phase region \(\text{Ce-35Fe-45Sb}\) (#11), \(\text{Ce-16Fe-48Sb}\) (#12) and \(\text{Ce-84Fe-10Sb}\) (#25)
B6 \((\text{FeSb}) + \tau_3 + (\alpha\text{Fe})\) three-phase region \(\text{Ce-72Fe-25Sb}\) (#1)
B7 \(\alpha\text{CeSb}_2 + \tau_1 + \text{Sb}\) three-phase region \(\text{Ce-8Fe-82Sb}\) (#14)
B8 \((\text{FeSb}) + \tau_1 + \text{FeSb}_2\) three-phase region \(\text{Ce-31Fe-65Sb}\) (#19)
B9 \(\tau_1 + \text{FeSb}_2 + (\text{Sb})\) three-phase region \(\text{Ce-23.53Fe-70.59Sb}\) (#21)
B10 \(\tau_3 + (\text{FeSb})\) two-phase region \(\text{Ce-47Fe-44Sb}\) (#24)

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2017.10.075.

Reference

[1] D.M. Zhu, C.L. Xu, C.R. Li, et al., Experimental study on phase relations in the Ce-Fe-Sb ternary system, J. Alloy. Compd. (2017), http://dx.doi.org/10.1016/j.jallcom.2017.09.276.