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Neutron diffraction study of the boride $\text{Y}(\text{Fe}_{11.04}\text{Ti}_{0.52}\text{B}_{0.43})\text{Ti}_{0.39}$: a new phase of a ThMn_{12} -type intermetallic interstitial compound

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Abstract. A sample with nominal composition $\text{YFe}_{10.5}\text{TiB}_{0.5}$ has been prepared through careful processing. X-ray diffraction analysis revealed that the main phase in the sample is in the tetragonal ThMn_{12} -type structure (space group, $I4/mmm$), and a small amount (less than 3%) of α -Fe exists as a second phase. Neutron diffraction measurements indicated that, in the tetragonal structure, the boron atoms occupy the 8i sites, substituting for a few Ti atoms, while the substituted Ti atoms enter the interstitial 2b sites. The real composition of the main phase was determined to be $\text{Y}(\text{Fe}_{11.04}\text{Ti}_{0.52}\text{B}_{0.43})\text{Ti}_{0.39}$.

1. Introduction

The structure and magnetic properties of ternary compounds of the type $\text{RFe}_{12-x}\text{M}_x$ ($\text{R} \equiv$ rare earth; $\text{M} \equiv \text{Ti}, \text{V}, \text{Cr}, \text{Mo}, \text{W}$, etc) have been studied by numerous investigators [1–4]. These compounds crystallize in the tetragonal ThMn_{12} structure in which there is only one crystallographic site for the rare earth and three non-equivalent sites for the M and Fe atoms. High Curie temperatures and high uniaxial anisotropies near room temperature make these systems promising starting materials for permanent-magnetic application [5, 6].

It has been discovered that the rare-earth–iron intermetallics of the $\text{RFe}_{12-x}\text{Ti}_x$ type can absorb moderate quantities of nitrogen [7]. Neutron diffraction measurements not only confirm that the nitrides maintain the tetragonal structure of their virginal compounds $\text{RFe}_{12-x}\text{Ti}_x$ but also indicate that the nitrogen atoms occupy the interstitial 2b sites, which leads to drastic changes in magnetic properties [7]. To date, the main disadvantage of the nitrated rare-earth–iron intermetallics is their thermal instability, which means they are easy to convert to RN_x and α -Fe phases at high temperatures.

In our previous work [8], we prepared various borides with the nominal composition $\text{RFe}_{12-x}(\text{Ti}, \text{V})_x\text{B}_y$, trying to investigate the effects of boron atoms in the ThMn_{12} -type rare-earth–iron intermetallics. Magnetic measurements, including high-field magnetization measurements and AC initial-susceptibility measurements, have shown that all the Curie temperatures, the iron moments and the anisotropies of the compounds undergo some changes upon the addition of boron [8]. Therefore, the position of boron atoms is the key to understanding the structure of the boride and interpreting the effects of boron on crystal-field and magnetic properties. In order to determine the positions of boron in these borides, we investigated the structure of $\text{YFe}_{10.5}\text{TiB}_{0.5}$ alloy by means of x-ray diffraction and neutron diffraction.

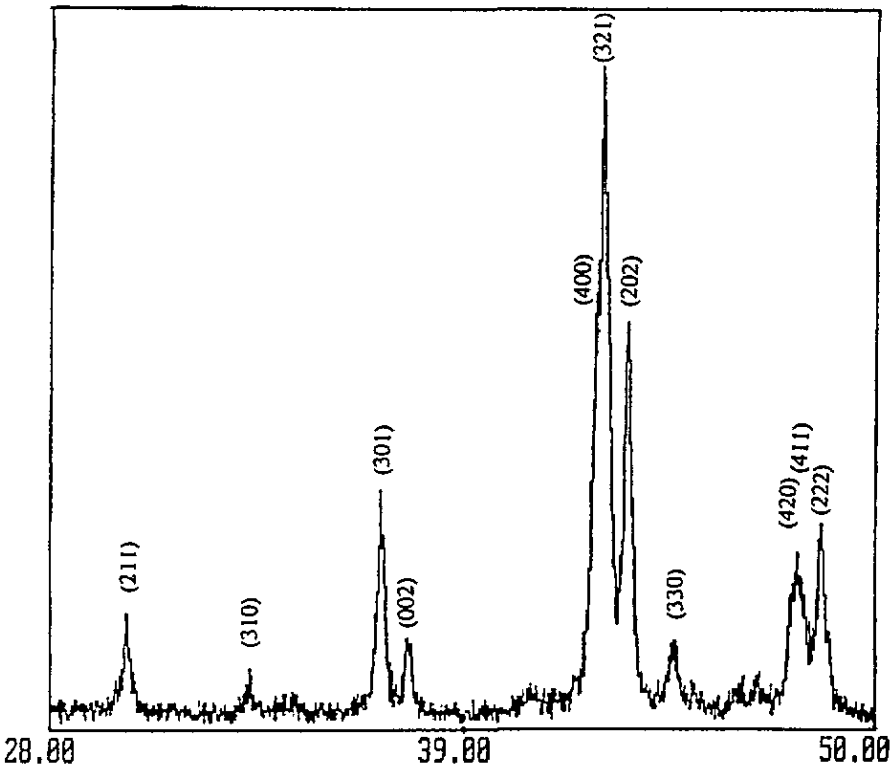


Figure 1. A part of the x-ray diffraction pattern of the $(YFe_{10.5}TiB_{0.5})$ sample.

2. Experimental details

The sample was prepared by arc melting the elemental constituents in a purified argon atmosphere, with the nominal composition $YFe_{10.5}TiB_{0.5}$; the melting point is $1286^{\circ}C$ (determined by the differential thermal analysis). To ensure homogeneity, the ingot was inverted and remelted. Then, the ingot wrapped in Mo foil was sealed in an evacuated quartz tube filled with high-purity argon and was annealed at $950^{\circ}C$ for 2 weeks, followed by rapid cooling to room temperature. The $ThMn_{12}$ -type structure of the main phase was identified using x-ray diffraction with $Cu K\alpha$ radiation.

Neutron diffraction measurements were performed on the powder diffractometer at the heavy-water research reactor at the Institute of Atomic Energy at Beijing. The powder sample was packed in a thin-wall cylindrical vanadium cell of 0.5 cm diameter and 5 cm high. The diffraction data were collected at room temperature with a neutron wavelength of 1.184×10^{-8} cm by scanning from $2\Theta = 10^{\circ}$ to 80° in steps of 0.15° . The diffraction patterns obtained were analysed by means of Rietveld's [9] profile technique. For the coherent scattering lengths, we used the values 0.7750×10^{-12} cm for yttrium, 0.9540×10^{-12} cm for iron, -0.3300×10^{-12} cm for titanium and 0.5300×10^{-12} cm for boron. Indication of the agreement between observed and calculated intensities, both nuclear and magnetic, is given by the discrepancy factor R_{total} :

$$R_{total} = \sum_i \left| S_i(\text{obs}) - \frac{1}{c} S_i(\text{calc}) \right| / \sum_i S_i(\text{obs})$$

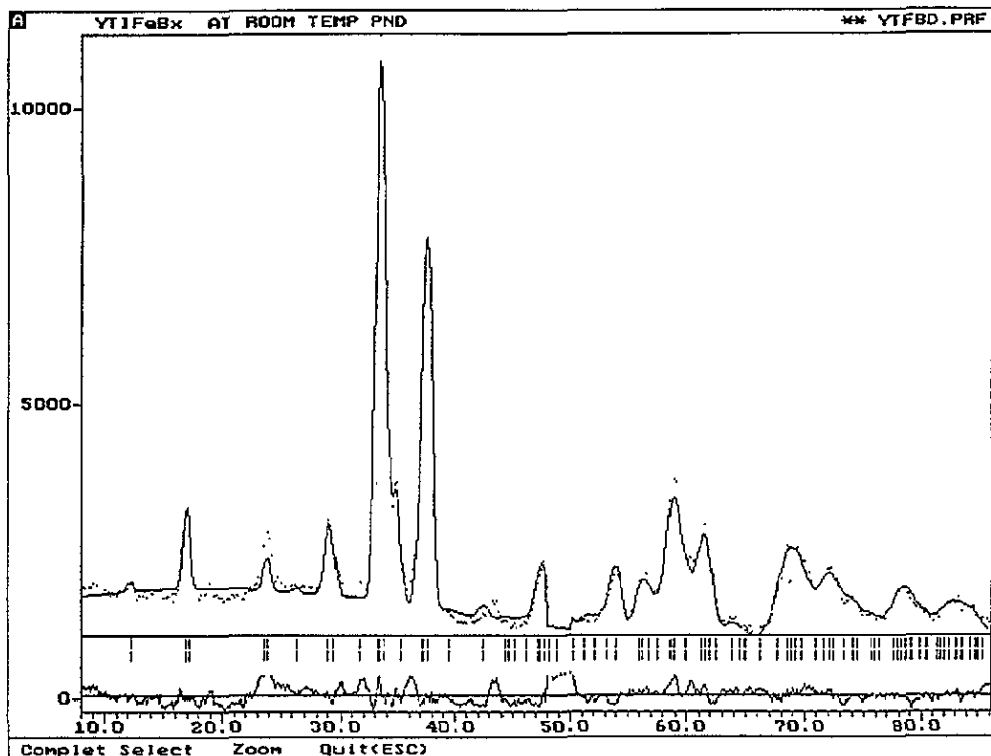


Figure 2. A part of the neutron diffraction pattern of the $(YFe_{10.5}TiB_0.5)$ sample.

where $S_i(\text{obs})$ and $S_i(\text{calc})$ are the observed and calculated integrated intensities, to be summed over all reflections, and c is a scaling factor. Similar expressions are used to obtain the separate R_{nuc} - and R_{mag} -values.

3. Results and discussion

The results of x-ray diffraction with $\text{Cu K}\alpha$ radiation are shown in figure 1. It is confirmed from the pattern that the main phase in the sample is of the ThMn_{12} -type structure, and there is a little α -Fe.

The neutron diffraction diagram obtained at room temperature is shown in figure 2. The observed diffraction lines are interpreted by nuclear and magnetic coherent scattering. The diffraction patterns of the sample can be indexed in a polyphase program, while the main phase is in a body-centred tetragonal cell (space group, $I4/mmm$), with parameters $a = (8.509 \pm 0.004) \times 10^{-8}$ cm and $c = (4.808 \pm 0.003) \times 10^{-8}$ cm.

The observed and calculated intensities for the sample are listed in table 1.

The results of the refinement procedure for the main phase, including the coordinates of the crystallographic sites, the occupancy factors for different atoms in these sites and the magnetic moments are given in table 2.

The position parameters for Y, Fe and Ti are very close to those obtained for $YFe_{11}Ti$ [10]. The Fe atoms are found to occupy the 8i, 8j and 8f sites, whereas the Ti atoms reside in the 8i sites. The most important result is the location of boron atoms, as shown in table 1.

Table 1. Calculated and observed intensities at 300 K.

$h k l$	2Θ (deg)	$I_{\text{calc}}(\text{nucl})$	$I_{\text{calc}}(\text{mag})$	$I_{\text{calc}}(\text{total})$	$I_{\text{obs}}(\text{total})$
2 0 0	15.996	694	48	742	742
1 0 1	16.261	212	10	222	183
3 0 1	28.048	910	9	919	953
0 0 2	28.514	377	0	377	505
4 0 0	32.315	2935	50	2985	3046
3 2 1	32.453	3884	43	3927	3993
2 0 2	32.862	2867	11	2878	2916
4 2 0	36.254	1919	40	1959	2030
4 1 1	36.379	1393	34	1427	1429
2 2 2	36.749	3934	28	3962	3851
4 4 0	46.351	490	3	493	431
5 2 1	46.453	115	0	115	103
4 2 2	46.757	411	1	412	394
3 0 3	50.212	275	0	275	283
5 1 2	51.169	238	0	238	195
6 2 0	52.208	186	1	187	161
6 1 1	52.301	185	0	185	160
3 2 3	53.042	1469	2	1471	1297
5 4 1	55.055	588	4	592	652
4 4 2	55.324	247	1	248	273
4 1 3	55.770	593	2	595	654
5 3 2	56.662	455	1	456	484
6 3 1	57.719	1516	4	1520	1600
6 0 2	57.980	1757	4	1761	1856
7 1 0	58.936	278	2	280	295
5 5 0	58.936	235	1	236	249
0 0 4	59.016	876	0	876	926
6 4 0	60.222	247	1	248	253
6 2 2	60.561	1535	4	1539	1530
7 2 1	62.830	367	0	367	433
7 3 0	63.988	117	0	117	186
7 1 2	66.753	437	1	438	452
5 5 2	66.753	372	0	372	384
8 0 0	67.637	888	1	889	898
6 5 1	67.716	120	0	120	121
6 4 2	67.955	925	1	926	952
6 1 3	68.351	112	0	112	118
4 0 4	68.905	1355	0	1355	1468
8 2 0	70.016	344	1	345	368
5 4 3	70.720	367	1	368	375
4 2 4	71.265	1034	1	1035	1013
7 3 2	71.503	191	0	191	183
6 6 0	72.360	184	0	184	165
6 3 3	73.054	975	1	976	870
8 3 1	74.750	471	0	471	440
5 1 4	74.745	119	0	119	111
8 4 0	76.962	603	0	603	603
8 2 2	77.264	433	0	433	427
7 2 3	77.641	255	0	255	245
4 4 4	78.168	406	0	406	379
5 3 4	79.299	244	0	244	228
6 6 2	79.529	178	0	178	166
7 6 1	81.554	320	0	320	302
9 3 0	82.600	169	0	169	165
6 2 4	82.669	160	0	160	157
3 2 5	83.337	631	0	631	658

Table 2. Coordinates of sites, occupancy factors for different atoms and magnetic moments in different sites. $a = (8.509 \pm 0.004) \times 10^{-8}$ cm; $c = (4.808 \pm 0.003) \times 10^{-8}$ cm. $R_{\text{nucl}} = 6.48\%$; $R_{\text{magn}} = 8.46\%$; $R_{\text{total}} = 5.51\%$.

Atom	Site	x	y	z	Number of atoms	μ_z (μ_B)
Y	2a	0.000 00	0.000 00	0.000 00	2.00	0.00
Fe	8i	0.356 10	0.000 00	0.000 00	6.09	1.83
Ti	8i	0.356 10	0.000 00	0.000 00	1.05	0.00
B	8i	0.356 10	0.000 00	0.000 00	0.87	0.00
Fe	8j	0.277 00	0.500 00	0.000 00	8.00	1.71
Fe	8f	0.250 00	0.250 00	0.250 00	8.00	1.66
Ti	2b	0.000 00	0.000 00	0.500 00	0.78	0.00

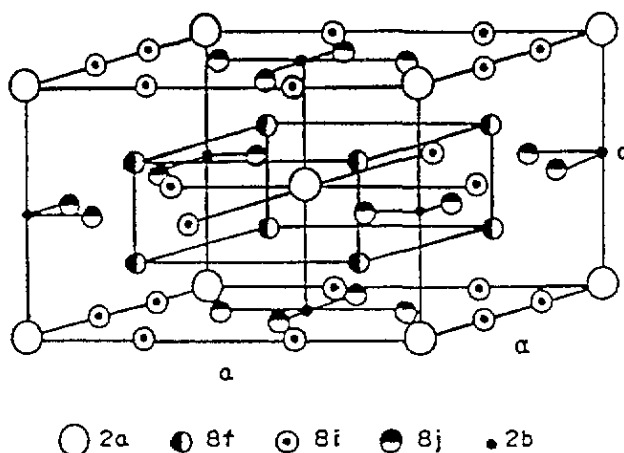


Figure 3. Schematic representation of the structure of $Y(Fe_{11.04}Ti_{0.52}B_{0.43})Ti_{0.39}$.

The boron atoms occupy the 8i sites, substituting for some of the Ti atoms. Surprisingly, it is found that the substituted Ti atoms can enter the interstitial position 2b, like nitrogen atoms. Thus the real formula composition of the main phase is $Y(Fe_{11.04}Ti_{0.52}B_{0.43})Ti_{0.39}$.

A schematic representation of the structure of $Y(Fe_{11.04}Ti_{0.52}B_{0.43})Ti_{0.39}$ is shown in figure 3.

From the analysis of our neutron diffraction data, it is believed that the B atoms take the substitution position and substitute for the transition-metal atoms which enter the interstitial position. The α -Fe content in the sample is about 3%.

We have examined in the same way another sample with the nominal composition $(YFe_{11}Ti_{0.8}B_{0.2})$ [11]. The results shows that the main phase also has the $ThMn_{12}$ -type structure, and the boron atoms prefer to occupy the substitution position, with the substituted Ti atoms in the 2b site. There is still a little α -Fe in the sample (less than 4%).

In conclusion, from the analysis of our neutron diffraction data, it can be derived that the boron atoms in the $ThMn_{12}$ -type intermetallics prefer to occupy the substitution position, totally different from the nitrogen atoms which occupy only the interstitial position. Meanwhile, it is found that the substituted transition-metal atoms can enter the interstitial position 2b. Therefore, this work will be helpful for understanding the structure of borides of $ThMn_{12}$ type and its relationship to the magnetic properties.

Acknowledgments

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