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A Mössbauer and structural study of disordered alloys $Fe_{3-x}Ti_xAl$ ($0 < x < 1$)

Krzysztof Brząkalik, Janusz E. Frąckowiak

Abstract A series of the disordered $Fe_{3-x}Ti_xAl$ (x = 0, 0.2, 0.45, 0.55, 0.65, 0.70, 0.75, 1) alloys obtained by arc-melting were studied. Directly after melting the samples were mechanically crashed and in that form examined by the structural and Mössbauer effect methods. The alloys were strongly disordered, but it was possible to identify, apart from Fe-bcc phase, the origins of forming such phases as Fe_2TiAl Heusler phase, Fe_3Al with DO_3 structure, FeAl and FeTi with B2 structure and non-stechiometric Fe_2Ti Laves phase with hexagonal C14 structure. For Ti concentration up to x = 0.45, the disordered Fe-bcc phase dominates. For Ti concentration from x = 0.55 to x = 1, the Fe_2TiAl phase coexists with FeAl phase (for x = 0.55, 0.65) and with FeTi phase (x = 0.7 and 0.75). In a sample with the nominal Fe_2TiAl composition of Fe_2TiAl Heusler phase, a non-stoichiometric Fe_2Ti Laves phase with hexagonal C14 structure was observed.

Key words Fe_2TiAl Heusler phase • Fe-Ti-Al system • Mössbauer spectroscopy

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Introduction

The Fe-Ti-Al alloys are interesting material for the sake of different structural and durability properties, in all concentration range of the components. Recently, in papers [4, 5, 7], the structure and mechanical properties of the Fe-rich alloys in such system were studied. At high temperatures microstructure of these alloys contains two or more phases: Fe-bcc, Fe_2Ti (Laves phase), Fe_2TiAl (Heusler phase) and $Fe_{0.5}Al_{0.5}$. Figure 1 shows part of the phase diagram of the Fe-Ti-Al system at 800°C, which was constructed on the basis of the diagram published in [5, 7]. The Fe-bcc phase region exists in the composition triangle spanned by the composition lines: Fe-Al-Fe_3Al, Fe_3Al-Fe_2TiAl and Fe_2TiAl-FeAl. There are two kinds of second-order order--disorder transitions in the Fe-bcc phase region A2/B2 and B2/DO_3, and two kinds of phase separations (A2 + B2) and (A2 + DO_3). The addition of Ti atoms to the Fe-Al system causes increasing of the order-disorder transition temperatures and expands the (A2 + DO_3) phase area [7]. In this paper, a series of the disordered alloys $Fe_{3-x}Ti_xAl$ (x = 0, 0.2, 0.45, 0.55, 0.65, 0.70, 0.75, 1) were investigated. In Fig. 1, these series are represented as a line A–B, on which the alloys are marked as short lines.

Experimental procedure

The investigated compounds $Fe_{3-x}Ti_xAl$ (x = 0, 0.2, 0.45, 0.55, 0.65, 0.70, 0.75, 1) were prepared as cast by arc melting in a high purity argon atmosphere. Directly after melting the samples were mechanically crashed and in that form examined by the structural and Mössbauer methods.

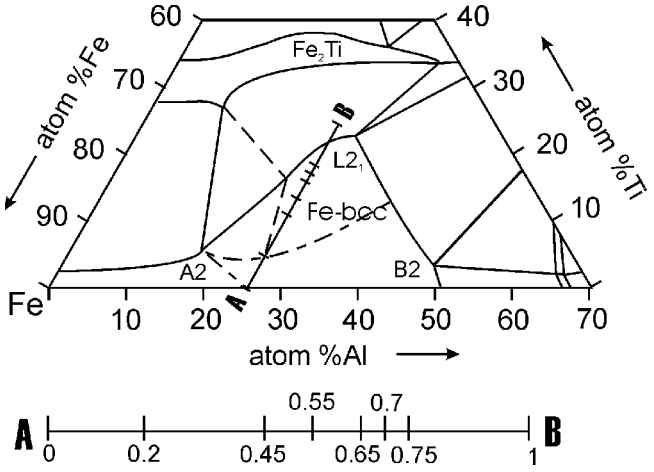

Fig. 1. A part of the phase diagram of the Fe-Ti-Al system at 800°C based on the diagram from papers [5, 7]. The line A–B represents the series of the alloys $Fe_{3-x}Ti_xAl$ examined in this work.

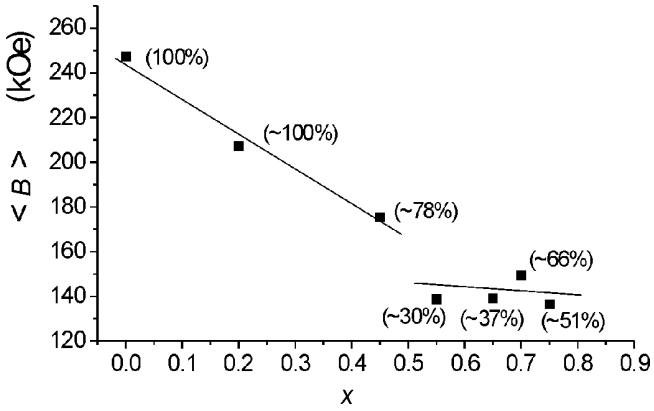

Fig. 3. Average hyperfine field <*B*> *vs.* Ti concentration (contribution of ferromagnetic phase given in parentheses).

The X-ray measurements were made at room temperature using a high-resolution Simens D-5000 diffractometer with filtered CuK_α radiation. The type of structure and lattice constant were determined.

The ^{57}Fe Mössbauer spectra were recorded at room temperature using a conventional constant acceleration spectrometer with a $^{57}Co(Rh)$ source with an activity of about 50 mCi. The isomer shift was determined relative to α-Fe at room temperature.

Results and discussion

The Mössbauer spectra of $Fe_{3-x}Ti_xAl$ compounds recorded at 295 K are shown in Fig. 2. To carry out the analyses, the ferromagnetic and paramagnetic parts were separated. The last one was described by the single lines and the quadrupole doublets. The changes in mean hyperfine field *vs.* the titanium concentration are shown in Fig. 3.

For samples with $x = 0$, 0.2 and 0.45, where ferromagnetic component dominates, these change are linear with slope $dB/dx = -158$ kOe. In this range of Ti concentration the lattice constant increases linearly (Fig. 4). The X-ray patterns and Mössbauer spectra are typical as for A2 structure, but more precision analyses for Fe_3Al and $Fe_{2.8}Ti_{0.2}Al$ show the presence of sextets with $B = 296$ kOe, typical for Fe atoms of DO_3 structure which has eight Fe atoms in the first shell and six Al atoms in the second one [1]. Such a mixture (A2 + DO_3) is possible and our results are in good agreement with phase diagram of the Fe-Ti-Al system [5, 7] at high temperatures. However, in the sample $Fe_{2.55}Ti_{0.45}Al$, apart from ferromagnetic contribution, about 18% of a paramagnetic component is observed. It was analyzed by superposition of three quadrupole doublets with parameters that are listed in Table 1. First of them, with the isomer shift IS = 0.03 mm/s, is connected with the formation of the Fe_2TiAl Heusler phase, the second one,

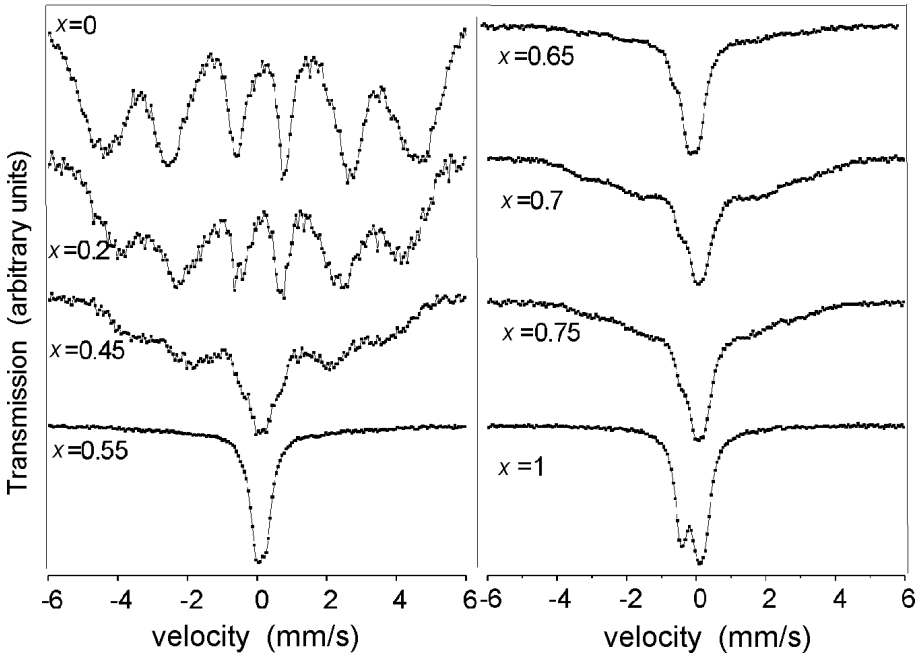

Fig. 2. Mössbauer spectra of $Fe_{3-x}Ti_xAl$ alloys at room temperature.

with IS = 0.14 mm/s, can be attributed to the Fe-Ti-Al solid solution, and the last one with IS = 0.28 mm/s corresponds to the FeAl phase [3].

In the $Fe_{2.45}Ti_{0.55}Al$ alloy, a strong reduction of ferromagnetic contribution is observed. According to paper [5] for such titanium concentration, liquid phase transforms directly in to the B2 structure. In quenched samples, the B2 structure is not formed; no superstructure lines in X-ray pattern are observed. But the rapid change in the lattice constant (Fig. 4) and the strong reduction of ferromagnetic part could point at a better order in these systems. Paramagnetic part of the Mössbauer spectra is described by means of two components: a single line (contribution about 37%) with IS = –0.025 mm/s and a quadrupole doublet (contribution about 32%) with IS = 0.246 mm/s. First of them corresponds to the Ti-rich Heusler Fe_2TiAl phase, and the second one is connected with the FeAl(Ti) phase.

In the $Fe_{2.35}Ti_{0.65}Al$ alloy, the contribution of the Fe_2TiAl phase decreased to 22%. In the Mössbauer spectra, an additional quadrupole doublet with IS = –0.107 mm/s and QS = 0.37 mm/s is observed, which is connected with formation of the FeTi single phase.

We observe no contribution of the FeAl(Ti) phase in the $Fe_{2.3}Ti_{0.7}Al$ and $Fe_{2.25}Ti_{0.75}Al$ alloys. Those alloys contain both Fe-bcc and Fe_2TiAl Heusler phases. An additional component (contribution about 5%) with IS = –0.106 mm/s for $x = 0.7$ and IS = –0.083 mm/s for $x = 0.75$ occurred, which was attributed to the FeTi phase.

The Mössbauer spectra for the nominal Fe_2TiAl composition can be described by one quadrupole doublet with IS = –0.096 mm/s and QS = 0.32 mm/s and a single line with IS = –0.004 mm/s. The first component is connected with the Fe_2Ti Laves phase with hexagonal C14 structure. The presence of this phase is confirmed by a structural investigation. Such structure has broad stability range up to the melting temperature [8]. This phase shows interesting magnetic properties. The planes of Fe atoms in the 6h sites have ferromagnetic interactions within each plane, but each 6h plane is coupled antiferromagnetically to the next 6h plane. The second Fe site (2a site) is located between the 6h planes and is paramagnetic. The stoichiometric Fe_2Ti is antiferromagnetic in the vicinity of the transition region from ferromagnetic to antiferromagnetic. Above the transition temperature ($T_N \sim 300$ K) it is paramagnetic and the Mössbauer spectra can be described by the quadrupole doublet with IS = – 0.296 mm/s and QS = = 0.39 mm/s [2, 6]. The doublet parameters of our sample differ a little from these, especially the value of IS, suggesting that the hexagonal phase in our sample is somewhat reacher than the pure Fe_2Ti Laves phase. In that situation, Ti atoms from 4f site are replaced by Fe atoms which causes a local reduction of the lattice constants with respect to pure Fe_2Ti [8]. It is also possible that the Fe_2Ti Laves phase contains Al atoms.

The second component of the Mössbauer spectra is connected with the disordered Fe_2TiAl alloy.

Table 1. Phase contribution (C), isomer shift (IS) (relative to α-Fe at room temperature), quadrupole splitting (QS) and phase description of paramagnetic part in Mössbauer spectra of $Fe_{3-x}Ti_xAl$ alloys.

x	C (at.%)	IS (mm/s)	QS (mm/s)	Phase description
0	–	–	–	–
0.2	–	–	–	–
0.45	8	0.03	0.45	Fe_2TiAl
	5	0.14	0.11	
	5	0.28	0.44	FeAl
0.55	37	–0.025	–	Fe_2TiAl
	32	0.246	0.017	FeAl(Ti)
0.65	8	–0.107	0.37	FeTi(Al)
	22	–0.069	–	Fe_2TiAl
	31	0.210	0.09	FeAl(Ti)
0.7	3	–0.106	0.380	FeTi
	36	0.06	–	Fe_2TiAl
0.75	6	–0.083	0.38	FeTi
	44	0.046	–	Fe_2TiAl
1	16	–0.004	–	Fe_2TiAl
	84	–0.096	0.32	non-stechiometric Fe_2Ti

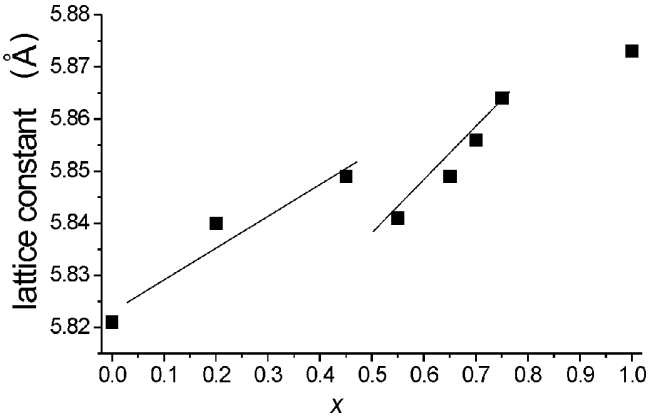

Fig. 4. Lattice constants of the $Fe_{3-x}Ti_xAl$ alloys as a function of Ti concentration (point for $x = 1$ corresponds to the Fe_2TiAl Heusler phase).

Conclusion

A series of the disordered alloys $Fe_{3-x}Ti_xAl$ ($x = 0, 0.2, 0.45, 0.55, 0.65, 0.70, 0.75, 1$) were investigated. Using the Mössbauer effect method we are able to describe the tendency of forming such phases as Fe_2TiAl, Fe_3Al, FeAl, FeTi and Fe_2Ti. In all ranges of Ti concentration we can single out few regions of different mixtures of intermetallic compounds. In the first region ($x = 0, 0.2, 0.45$), the alloys contain mainly the Fe-bcc phase with a small amount of the Fe_3Al phase. The average hyperfine magnetic field decreases linearly with Ti concentration. In the next region ($x = 0.55, 0.65$), the alloys contain mainly the paramagnetic Fe_2TiAl and FeAl phases. Also a small amount of FeTi phase occurs. In the last region ($x = 0.7, 0.75$ and 1), the alloys contain the Fe_2TiAl Heusler and FeTi phases. For the Fe_2TiAl nominal composition, the non-stoichiometric Fe_2Ti Laves phase with hexagonal C14 structure is visible. The determined sequence of the phases corresponds to the equivalent phase diagrams at high temperatures.

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