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Point defect structure in B2-ordered Fe–Al alloys

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ABSTRACT

In this work, Mössbauer spectroscopy and X-ray powder diffraction (XRD) have been employed to study various types of the point defect formation in B2-structured intermetallic phases of the Fe–Al system as a function of Al concentration. We present the values of the ^{57}Fe isomer shift and quadruple splitting for the components describing the point defect in the local environment of a Mössbauer nuclide. The concentrations of Fe vacancies and anti-site Fe atoms substituting Al (Fe-AS) are determined. The results show that an increase in Al content causes an increase in vacancy and Fe-AS concentrations.

1. Introduction

Iron aluminides represent an intriguing class of new materials: they offer a good combination of mechanical properties, as high specific strength/weight ratio, excellent corrosion and oxidation resistance and low raw material costs [1–3], which make them potential candidates for the substitution of ferrite stainless steel in applications at moderate to high temperatures. The extensive technological application of iron aluminides, however, is impaired by their low room temperature tensile ductility. The development of new, more ductile Fe–Al alloys depends on a thorough understanding of their deformation mechanisms in relation to the defect structure in these materials. Experimental as well as theoretical studies [1–6,9,10,12–19] suggest that point defects in iron aluminides present a complex structure, especially of triple defect type.

This paper describes the Mössbauer spectroscopy and X-ray powder diffraction (XRD) studies of point defect formation in FeAl B2-structured intermetallic phases of the Fe–Al system. Mössbauer spectra are analyzed using a model [9] according to which the vacancies in the Fe-sublattice and Fe anti-site atoms substituting Al (Fe-AS) in atomic shells close to the probe atom, influence the isomer shift and quadrupole splitting of individual spectrum components. The concentrations of point defects are determined from the intensities of these components and they are correlated with changes in the Al content.

2. Experimental details

The chemical compositions of the investigated alloys are presented in Table 1. The samples were obtained from Armco iron, aluminum of 99.99% purity, and small amounts of other additives (Mo, Zr, B and C) in order to improve the thermal and mechanical properties of the alloys. The ingots were prepared by melting using spinel $Al_2O_3 \times MgO$ crucibles in an induction furnace at 10^{-2} torr. The ingots were re-melted three times to insure homogeneity, and they were annealed in a vacuum furnace for 48 h and then cooled down slowly in the furnace. The phase analysis was carried out by applying X-ray diffraction using a X-ray Philips diffractometer equipped with graphite monochromator using Cu K-α radiation on rotating samples. The selected X-ray diffraction patterns are presented in Fig. 1. The features of B2-type structure prevail in the diffraction spectra. Lattice constant parameters and long-range order parameters determined by Rietveld refinement method show a tendency to increase with an increase in aluminum contents in the samples. The ^{57}Fe Mössbauer spectra were recorded in transmission geometry at room temperature by means of a constant-acceleration spectrometer of the standard design. The 14.4 keV gamma rays were provided by a 50 mCi source of ^{57}Co/Rh. Hyperfine parameters of the investigated spectra are related to the α-Fe standard. The experimental spectrum shape was described with a transmission integral calculated according to the numerical Gauss–Legandre's procedure [11] which enables the determination of real intensities of the as fitted components.

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Table 1
Chemical compositions of the investigated materials [at.%].

Contents [%]	I	II
Fe	61.64	54.64
Al	38	45
Additions	Mo – 0.20; Zr – 0.05; C – 0.1; B – 0.01	

3. Results and discussion

The selected Mössbauer spectra are presented in Fig. 2. All Mössbauer spectra were fitted using the model proposed by Bogner et al. [7]. The Mössbauer spectrum of the $Fe_{55}Al_{45}$ sample fitted with this model is shown in Fig. 2. According to this model, the spectrum contains four components describing different local environments of a ^{57}Fe nuclide. The first component (I) – a single line – represents an ordered B2 structure. The second component (II) – a single line (which approximates an unresolved quadruple doublet) – relates to the case when the Mössbauer Fe nuclide is located in a corner of the cubic centered unit cell, and an Fe-AS atom is situated in the center of this unit cell. The third component (III) – a doublet of lines (which approximates an unresolved Zeeman sextet) – corresponds to a Fe atom located in the Fe-AS position. The fourth component (IV) – also a quadruple doublet of lines – represents the case of a vacancy in the near Fe surrounding.

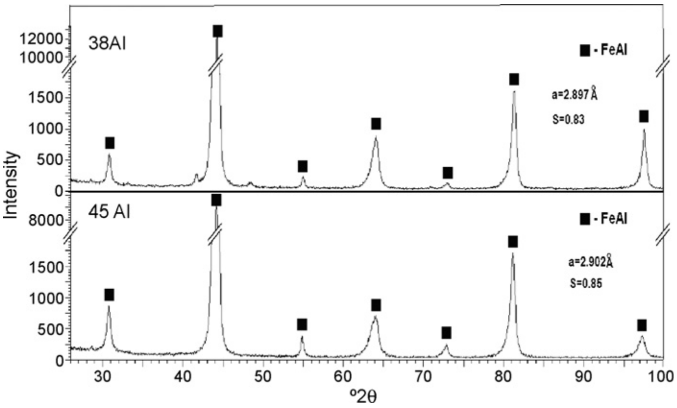

Fig. 1. X-ray diffraction patterns of $Fe_{62}Al_{38}$ and $Fe_{55}Al_{45}$ samples annealed at 1000 °C for 48 h.

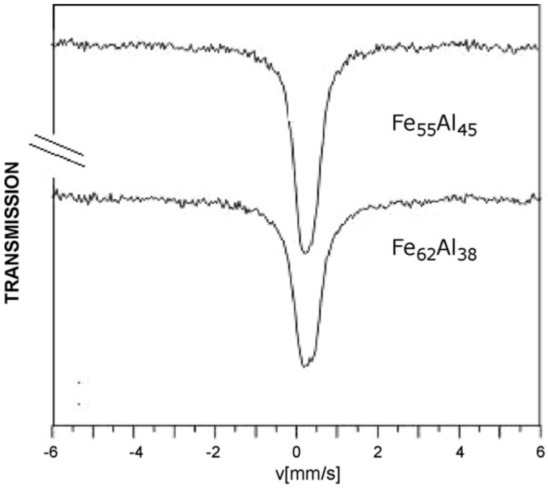

Fig. 2. The ^{57}Fe Mössbauer transmission spectra for investigated alloys.

Table 2
Values of the hyperfine parameters (IS, QS) and A – sub-spectra area.

Samples	Component	IS[a,b] [mm/s]	QS[a] [mm/s]	A [%]
$Fe_{63}Al_{38}$[b]	L-I	0.19		83
	L-II	0.06		14
	Q-III	0.04	0.25	1.9
	Q-IV	0.23	0.13	1.1
$Fe_{55}Al_{45}$[b]	L-I	0.24		85
	L-II	0.07		11.7
	Q-III	0.05	0.22	2.1
	Q-IV	0.21	0.17	1.2

[a] Error estimated from the fitting procedure is equal ±0.005.
[b] Relative to the α-Fe foil at room temperature.

Table 3
Values of vacancy and anti-site atom Fe-AS concentrations in the samples of B2-ordered FeAl determined by Mössbauer spectroscopy investigations.

Estimated phase composition	Vacancy concentration V_{Fe} [%][a]	Concentration Fe-AS [%][b]
$Fe_{62}Al_{38}$	0.04	1.9
$Fe_{55}Al_{45}$	0.05	2.1

[a] Error estimated is equal to ±0.006.
[b] Error estimated is equal to ±0.05.

Table 2 presents the evolution of the isomer shift (IS) values and quadruple splitting (QS) of the spectra components depending on the aluminum concentration. Similar values of the IS and QS for the components describing the ordered B2 structure and the point defect which revealed in theoretical calculations [20] and experiments [8–9,12,16–17]. The values of vacancy and anti-site atom concentrations found using the described model are shown in Table 3. In order to estimate the concentration of vacancies in the Fe-sublattice, the intensity of a sub-spectrum was divided by 26 [9]. The obtained values of vacancy concentrations and Fe-AS show an increase with increasing Al content, confirming the results of theoretical calculations [13] and some experimental data [9,10,16–17,19]. According to the literature [3–6,9,10,12,14], the vacancies in the Fe-sublattice V_{Fe} are the dominant type of point defects in B2 FeAl alloys (may be organized in triple defects, i.e. two vacancies and an anti-site atom [5,10]). Vacancy formation in Fe-rich Fe–Al alloys has been studied by Schaefer et al. [19] using the positron lifetime technique. They found that the thermal vacancy concentration is about 2.3×10^{-5} at 600 °C, increasing to about 1.3×10^{-3} at 900 °C. We also carried out a study of vacancies formation in alloys I and II (see Table 1) as a function of Al concentration [19]. The results show that the total concentration of point defects is so high that the positrons were exclusively trapped. In alloys with more then 38% Al, vacancies in the Al sublattice (V_{Al}) are formed in a minor amount, in comparison to the vacancies in the Fe-sublattice (V_{Fe}). The values of vacancies concentrations in the samples containing microadditions (I and II – see Table 1), estimated in this work, are slightly lower than vacancies concentrations in Fe_xAl_{1-x} ($x > 0.5$) alloys, calculated and reported in [13] and those of experimental data published in [9,10].

Those results were correlated to the electron structure modification in the examined materials by the microadditions. Such a character of the defect structure, mainly the lower concentration of vacancies in the alloys modified by microadditions, confirms the advisability of their introduction in order to improve plasticity of these materials.

4. Conclusions

Point defect concentrations in a series of intermetallic B2-ordered FeAl alloys were determined by applying Mössbauer spectroscopy. It was found that the investigated materials contain high concentrations of point defects, which significantly increase with an increase in aluminum content. The values of the vacancies concentrations in the Fe_xAl_{1-x} ($x > 0.5$) samples containing microadditions, estimated in this work, are slightly lower than vacancies concentrations in the Fe_xAl_{1-x} ($x > 0.5$) alloys determined by other authors. Such a change in the defect structure – mainly the lower concentration of vacancies in the alloys modified with microadditions – confirms the advisability for improving the plasticity of these materials.

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