Proceedings of the All-Polish Seminar on Mössbauer Spectroscopy, Warsaw, Poland, June 18–21, 2010

Effect of Annealing in Multicomponent bcc Alloys

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Multicomponent single phase alloys were synthesized according to the idea of iron-average atom system. X-ray diffraction shows formation of bcc phase and traces of unidentified phase. Mössbauer spectra indicate presence of two components with different hyperfine magnetic field distributions. The high field component corresponds to the majority ferromagnetic phase. Few per cent of iron builds low field component. The dominant effect of annealing consists in an increase of the low field component.

PACS: 71.20.Be, 76.80.+y, 61.05.Qr, 61.50.Ks, 81.30.Hd

1. Introduction

One of the methods of systematic changing of physical properties of the crystalline phase is doping or alloying. However, the changes of chemical composition of some simple systems lead to appearance of additional crystallographic phases or segregation of composition — in other words non-homogeneity of the system [1]. On the other hand, the Gibbs phase rule allows formation of $n+1$ phases in n component system at constant pressure [2]. Usually smaller number of different phases is observed [3]. Indeed, the authors of [3] reported ssuccessful synthesis of equiatomic multicomponent single fcc metallic phase [3].

Let us consider an example of Al or Si diluted in Fe matrix. At small concentrations $Fe_{1-x}Al_x$ is disordered and has bcc structure. At higher concentrations, local nearest neighbour environment is, on the average, cubic, however DO_3 and/or B2 superstructures are formed. Similar behaviour is observed in $Fe_{1-x}Si_x$, but in contrast to Fe-Al, at concentration $x \sim 0.3$ another crystallographic phase, B20, is formed [4] with local environments and packing ratio quite different from these ones in bcc structure. The main idea of present study consists in introducing systematic structural changes based on so called average atom approach. A few elements added to Fe matrix, in considered examples Al and Si, will increase configurational entropy. It may be expected that a mixture of various added elements (called an average atom) will weaken the tendency to form local ordering and will thus extend the stability range of the matrix phase (in considered case bcc).

The paper presents effect of annealing on the bcc Fe based system with average atom formed by A=(Al, Si, V, Cr).

2. Samples and X-ray examination

The appropriate amounts of elements of purity better than 99.998% were prepared, melted and three times remelted in an arc furnace to get homogenous ingots. Composition of the samples are given in Table. Part of as cast samples were grinded to powders. Other part of the samples were annealed for 72 h at $T = 800$ °C and then grinded to powders. The structure of the samples was checked by X-ray measurements. All the samples with concentration of average atom up to $x_A = 0.4$ exhibit the single bcc phase. The sample with concentration $x_A = 0.5$ shows less than 20% of an extra bcc phase with different lattice parameter. Composition dependence of the lattice parameters are shown in Fig. 1 and in Table. The measurements indicate that annealing process does not affect the values of lattice parameters.

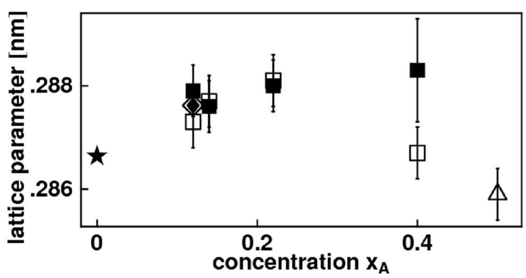

Fig. 1. Concentration dependence of lattice parameter for as cast (empty symbols) and annealed (full symbols) samples. Abbreviation of the symbols is shown in Table. Empty and full diamond symbols overlap. Star symbol corresponds to pure α-Fe.

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TABLE

Compositions and lattice parameters of the samples studied.

symbol in Fig. 1	concentration of average atom x_A	Lattice parameter [nm]		concentration of elements				
		as cast	annealed	Fe	Al	V	Si	Cr
box	0.12	0.2873(5)	0.2879(5)	0.880	0.036	0.054	0.030	0
box	0.14	0.2877(5)	0.2876(5)	0.860	0.042	0.063	0.035	0
box	0.22	0.2881(5)	0.2880(5)	0.780	0.066	0.099	0.055	0
box	0.40	0.2867(5)	0.2883(10)	0.60	0.12	0.18	0.10	0
diamond	0.12	0.28762(9)	0.28762(9)	0.880	0.035	0.053	0.029	0.003
triangle	0.50	0.2859(5)	—	0.50	0.125	0.125	0.125	0.125

3. Mössbauer measurements

The absorbers were prepared by covering of double sided scotch tape by powdered sample. Appropriate number of such layers were collected to form absorber of thickness of between 10 and 15 mg of Fe/cm^2. Mössbauer measurements were performed at room temperature. Calibration spectrum of α-Fe foil is shown as the uppermost spectrum of Fig. 2a. Further experimental details can be found elsewhere [5]. The spectra (Fig. 2a) show broad, six line pattern typical for ferromagnetic disordered systems, like amorphous ferromagnets or disordered binary or ternary alloys. We do not observe features like two Zeeman sextets that are typical for ordered DO_3-type of Fe_3Si or Fe_3Al structures. Some absorption is observed in the zero velocity region. Its intensity increases after annealing, compare spectra abbreviated by 12 and 12a at $v = 0$ mm/s in Fig. 2a.

All spectra were successfully fitted by two components offered in NORMOS package in thin absorber approximation. The first, dominant component is due to continuous distribution of hyperfine magnetic field, see example in Fig. 2c, which corresponds to broad six absorption lines shown in Fig. 2b by red line. The second component corresponds to a Gaussian distribution of hyperfine magnetic field, see green line in the example in Fig. 2b. For both components zero quadrupole splitting was assumed. All fits are of good quality as in the presented example, Fig. 2b. In the case of poorly resolved spectra of $x = 0.4$ sample, the parameters of Gaussian component were extrapolated and fixed during the fits.

The main component shows parameters dependent monotonically on the composition of average atom, see Figs. 3a–b. For the low field component no systematic dependence of the parameter on composition was found. The average isomer shift is between 0.36 mm/s and 0.48 mm/s, the mean value of the hyperfine field distribution is between 4.4 T and 4.9 T and the standard deviation of the distribution is in the range 0.9–1.2 T. The relative area of the low field component increases approximately twice after annealing and is always below 10% for samples investigated so far.

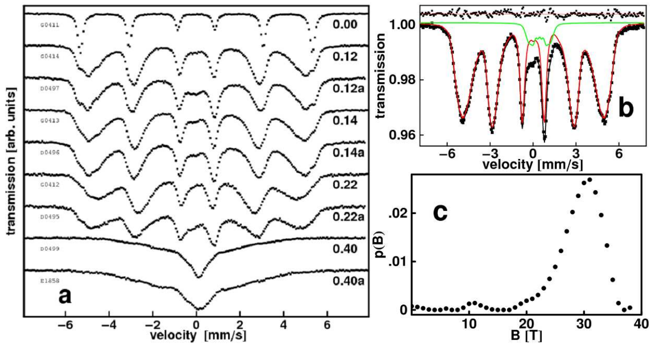

Fig. 2. a) Evolution of Mössbauer spectra measured at room temperature for multicomponent as cast and annealed (abbreviated by "a") alloys. Numbers on the right correspond to concentration of the average atom, as in Table. b) Example of data analysis for $x = 0.14$ sample. Red line corresponds to the distribution of hyperfine magnetic field in high field region while green line to the Gaussian distribution in low field region. See text. c) Distribution of hyperfine magnetic field of high field part, shown in (b) by red line.

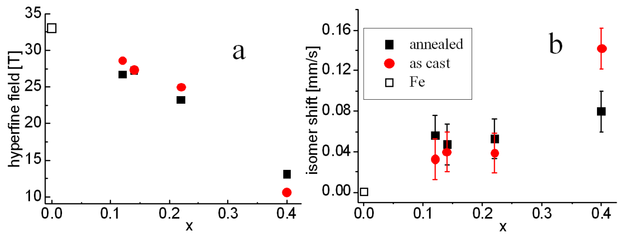

Fig. 3. a) Average hyperfine magnetic field and b) isomer shift for as cast and annealed samples. The averages correspond to the both high and low field components.

4. Discussion and conclusions

X-ray diffraction patterns show formation of the bcc matrix, irrespectively of applied annealing procedure. Most of iron forms typical for disordered ferromagnets single peak in the distribution of hyperfine magnetic field (Fig. 2b). Few per cent of iron belongs to the low field part. Large isomer shift indicates that local iron environments are enriched in Al and Si, the elements which enhances isomer shift of iron in bcc (and originating from bcc superstructures: DO_3, B2) alloys. Result of fits indicate that in the investigated concentration range the low field phase is characterized by almost constant and clearly nonzero hyperfine magnetic field. Our results are consistent with the interpretation that low field phase originates from (Al-Si)-rich inhomogeneities or fluctuations for which magnetic order is different from that one of the main matrix, while crystal structure remains bcc. Annealing process causes further segregation of the atoms changing short range order and formation of Fe environments characteristic for ordered Fe_3Al, Fe_3Si and FeAl alloys.

Acknowledgements

The work was partially supported by funds allocated for scientific research for the years 2008–2011 as a research project NN202172335.

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