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The Crystal Structure and Magnetic Properties of Selected fcc FeNi and $Fe_{40}Ni_{40}B_{20}$ Alloys

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The crystal structure and magnetic properties of polycrystalline alloys $Fe_{62.5}Ni_{37.5}$, $Fe_{60}Ni_{40}$, $Fe_{50}Ni_{50}$ obtained by arc-melting and $Fe_{40}Ni_{40}B_{20}$ alloy obtained by melt spinning technique were investigated by X-ray, magnetostatic and Mössbauer effect methods. The X-ray measurements show that $Fe_{40}Ni_{40}B_{20}$ alloy has a face-centered structure (fcc) which means that boron did not cause an amorphous rendering. The lattice constants for this alloy ($a = 3.53$ Å) is smaller than for FeNi alloys ($a > 3.57$ Å) which suggests that boron atoms were built-in in the crystal lattice. The Curie temperature of this alloy is more than 150 K higher in comparison with the of FeNi alloys, but the magnetic moment connected with this alloy is more than 0.17 μ_B/atom smaller than the magnetic moments of FeNi alloys. The shape of hyperfine field distribution for $Fe_{40}Ni_{40}B_{20}$ is similar to the shape of hyperfine field distribution for the investigated fcc $Fe_{62.5}Ni_{37.5}$ alloy, but both are different from another investigated hyperfine field distribution of FeNi alloys.

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1. Introduction

The FeNi alloys attract the intense attention of investigators due to their numerous applications (laser cavity construction, dimensional stabilizers, super-tanker construction, etc.) and due to anomalies of some physical properties which take place when the iron concentration changes between 60% to 70% (invar region). The FeNi alloys, depending on nickel concentration and thermal treatment can crystallize in bcc and fcc structures. Alloys with fcc structure exhibit very interesting thermal and magnetic properties such as: nearly zero thermal expansion coefficient around room temperature, sudden deviation of the saturation magnetization from the Slater–Pauling curve, strong forced volume magnetostriction, low ferromagnetic ordering temperature T_c compared to the T_c of bcc iron and fcc nickel and non-Invar γ-FeNi. These properties strongly depend on nickel concentration, temperature and preparation method [1]. Therefore, they have been the object of many experimental and theoretical works [2–4].

In this paper we will present the results of X-ray, magnetic and Mössbauer effect measurements for $Fe_{62.5}Ni_{37.5}$, $Fe_{60}Ni_{40}$, $Fe_{50}Ni_{50}$ and $Fe_{40}Ni_{40}B_{20}$ alloys. We want to check how replacement iron by boron atoms influences crystal and magnetic properties Fe–Ni alloys.

2. Experimental

The polycrystalline $Fe_{62.5}Ni_{37.5}$, $Fe_{60}Ni_{40}$, and $Fe_{50}Ni_{50}$ alloys were prepared by arc-melting stoichiometric quantities of the starting metals in an argon atmosphere. The ingots were re-melted several times to ensure homogeneity. The investigation was made on powdered samples of FeNi with granule sizes smaller than 30 μm made by grinding on diamond file. The $Fe_{40}Ni_{40}B_{20}$ alloy was obtained by a melt spinning technique used for the rapid cooling of liquids [5], and the alloy was a ribbon with a thickness of about 400 μm.

X-ray diffraction studies (XRD) of the investigated FeNi alloys were performed at room temperature using a Siemens D5000 X-ray diffractometer and Cu K_α radiation.

The magnetic measurement of the investigated samples was performed at temperatures up to 800 K in magnetic fields up to 1.2 T using the Faraday method.

The Fe^{57} Mössbauer spectra were recorded at room temperature using a constant acceleration spectrometer with Co^{57}:Pd source. Metallic iron powder was used for velocity calibrations of the Mössbauer spectrometer. The obtained spectra were fitted as a superposition of several Zeeman sextets and single lines by means of a hyperfine field distribution method.

3. Results and discussion

The X-ray diffraction measurements showed that the investigated FeNi alloys were single face-centered cubic phases (fcc). The $Fe_{40}Ni_{40}B_{20}$ has a fcc structure, which means that the boron did not cause the amorphous rendering and partially diffused to the FeNi fcc structure. Figure 1 shows X-ray diffractograms for investigated compounds.

In the XRD diffraction pattern of the $Fe_{40}Ni_{40}B_{20}$ alloy, only some planes with the Miller indices were observed. Detailed analysis of diffraction patterns indicated that the [111] plane is parallel to the ribbon surface and

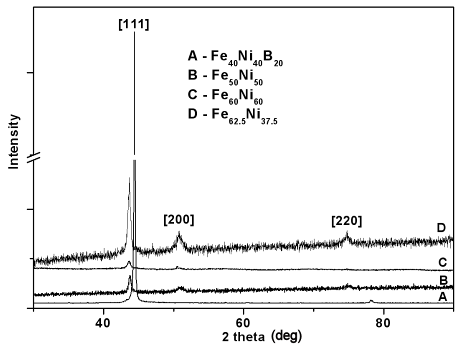

Fig. 1. The XRD diffraction patterns of $Fe_{40}Ni_{40}B_{20}$ and investigated FeNi alloys.

was not observed in diffraction pattern peak from precipitate boron or other phases. Results of crystallographic and magnetic measurements are presented in Table I. As follows from this table, the lattice constant of the $Fe_{40}Ni_{40}B_{20}$ alloy is smaller than the lattice constants of metallic Ni and investigated fcc FeNi alloys. The atomic radius of boron is almost twice smaller than the atomic radius of iron or nickel. Therefore, smaller lattice parameter for $Fe_{40}Ni_{40}B_{20}$ alloy is a result of replacement, by small boron atoms, of some places of iron atoms in fcc FeNi crystal lattice. –

TABLE I

Lattice constant a, magnetic moment μ at room temperature and the Curie temperature T_c for the investigated compounds and nickel.

Compound	a [Å]	T_c [K]	μ [μ_B/atom]
Ni	3.516	640	0.606
$Fe_{62.5}Ni_{37.5}$	3.599	417	1.57
$Fe_{60}Ni_{40}$	3.588	515	1.74
$Fe_{50}Ni_{50}$	3.578	540	1.35
$Fe_{40}Ni_{40}B_{20}$	3.530	680	1.18

Magnetic studies show that the investigated compounds are ferromagnetic with a Curie temperature above room temperature (Table I). The Curie temperature of the $Fe_{40}Ni_{40}B_{20}$ alloy is more than 150 K higher in comparison with this of FeNi alloys, but the magnetic moment connected with this alloy is more than 0.17 μ_B/atom smaller than the magnetic moments of FeNi alloys. Smaller value of magnetic moment $Fe_{40}Ni_{40}B_{20}$ alloy in comparison with investigated FeNi alloys arises from smaller value of iron concentration in this alloy. The increase of the Curie temperature with increasing boron concentration was observed in amorphous iron alloys with boron [6, 7]. It can be explained in terms of the two spin states model first proposed by Weiss [8].

Weiss assumed that Fe atoms in fcc like neighbourhood can exist in two magnetic states: low spin states with magnetic moment 0.5 μ_B and high spin states with magnetic moment 2.8 μ_B. These two states are separated energetically and the value of ΔE for pure gamma iron is equal to -0.0355 eV. When nickel concentration increases in FeNi alloys, ΔE passes through zero and becomes positive, then ferromagnetic high spin state of iron with high T_C dominates. It was found [6] that in amorphous Fe–B alloys ΔE increases with increase of boron concentration in alloy and hence the Curie Temperature as an increasing function of the separation energy ΔE increases.

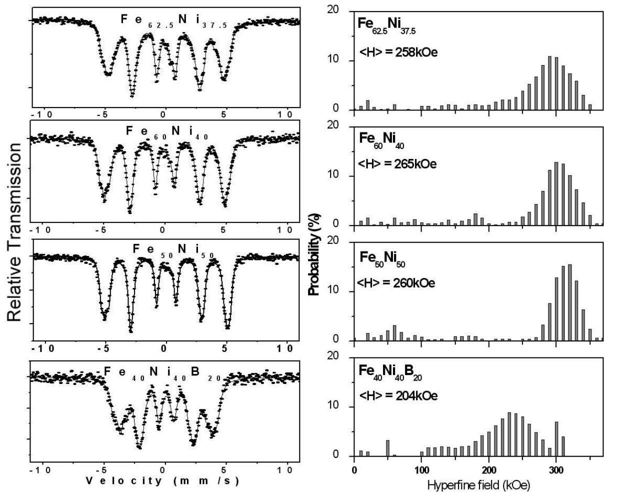

Fig. 2. The Mössbauer spectra and respective hyperfine field (HF) distribution for the investigated compounds at room temperature.

The Mössbauer absorption spectra and diagrams of hyperfine field (HF) distributions are presented in Fig. 2. The fitting parameters of the Mössbauer spectra are presented in Table II. The hyperfine field distributions for investigated alloys are broad, this is connected with different local surroundings of the Fe atom in fcc lattice. We suppose that the hyperfine fields larger than those for pure iron are the effect of surrounding the Fe atom by zero to nine Fe atoms in the first coordination sphere. Hyperfine fields smaller than about 50 kOe are connected with Fe atoms surrounded by ten to twelve other Fe atoms [9]. The hyperfine field distribution for $Fe_{40}Ni_{40}B_{20}$ is also broad, and the average value of the hyperfine filed is smaller than for FeNi alloys, it is probably connected with a statistical location of boron atoms in the fcc structure. This statistical location of boron in the crystal lattice leads to increasing number of different crystallographic and magnetic positions of Fe atoms. Hence the hyperfine field distribution is broader than for FeNi alloys. The hyperfine field distributions for $Fe_{60}Ni_{40}$, and $Fe_{50}Ni_{50}$ alloys are narrow in comparison to another two alloys and arise from reduction of statistically not equivalent crystallographic position Fe atoms in fcc crystal lattice.

The smaller magnetic moment and average value of hyperfine field distribution in $Fe_{40}Ni_{40}B_{20}$ alloy in

TABLE II

The fitting parameters of Mössbauer spectra: hyperfine magnetic field H_{hf}, isomer shift IS, and the percentage contribution of components in the spectrum for investigated compounds.

Sample	H_{hf} [kOe]	IS [mm/s]	Contribution [%]
$Fe_{62.5}Ni_{37.5}$	256	0.009	27
	285	0.034	25
	303	0.035	21
	325	0.041	23
$Fe_{60}Ni_{40}$	286	0.024	35
	307	0.019	36
	328	0.021	27
$Fe_{50}Ni_{50}$	298	0.031	30
	315	0.031	38
	331	0.026	31
$Fe_{40}Ni_{40}B_{20}$	202	0.113	33
	233	0.121	45
	264	0.048	23

comparison with these values of FeNi alloys can arise not only from smaller concentration of Fe atoms but also from reduction of magnetic moment on nickel atom in presence of boron atoms. Such effect was observed in amorphous $(Fe_{1-x}Ni_x)_{80}B_{20}$ $(0.1 < x < 1)$ alloys [10].

4. Summary

Introduction of boron atoms into a fcc FeNi crystal lattice leads to the reduction of magnetic moment, increase Curie temperature, and broadening of the hyperfine field distribution. We assume that those results were consequences of the fact that boron atoms occupy a statistical position in the crystal lattice similar to that in amorphous Fe–B alloys.

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