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Mössbauer effect studies of $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ compounds

Agata Jabłońska, Jan Suwalski, Paweł Stoch, Jarosław Pszczoła, Piotr Guzdek, Paweł Szamański, Antoni Pańta

Abstract. A consequence of the Fe/Ni substitution in the $Dy(Fe_{0.4}Co_{0.6})_2$ compound was studied in the present paper. For this purpose the synthesis and X-ray analysis (295 K) of the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series were performed. The cubic, $MgCu_2$-type, *Fd3m* crystal structure was observed across the series. ^{57}Fe Mössbauer effect spectra for the series were collected at 77 K. The obtained crystallographic data and the hyperfine interaction parameters are presented. The magnetic hyperfine fields form a separate branch of the Slater-Pauling curve known for the $Dy(Mn_{1-x}Fe_x)_2$ and $Dy(Fe_{1-x}Co_x)_2$ series. The data are qualitatively related to the Stoner model.

Key words: crystal structure • Mössbauer effect • hyperfine interaction • Slater-Pauling curve • band structure

A. Jabłońska✉, J. Suwalski
Nuclear Methods of Solid State Physics Department,
Institute of Atomic Energy,
05-400 Otwock-Świerk, Poland,
Tel.: +48 22 7180155, Fax: +48 22 7793888,
E-mail: a.jablonska@cyf.gov.pl

J. Pszczoła, P. Guzdek, P. Szamański
Department of Nuclear Methods,
AGH University of Science and Technology,
30 A. Mickiewicza Ave., 30-059 Kraków, Poland

P. Stoch
Nuclear Methods of Solid State Physics Department,
Institute of Atomic Energy,
05-400 Otwock-Świerk, Poland
and Faculty of Materials Science and Ceramics,
AGH University of Science and Technology,
30 A. Mickiewicza Ave, 30-059 Kraków, Poland

A. Pańta
Department of Metallurgy and Materials Engineering,
AGH University of Science and Technology,
30 A. Mickiewicza Ave., 30-059 Kraków, Poland

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Introduction

Magnetic properties and hyperfine interactions of the rare earth-transition metal compounds are mainly governed by the 3*d* electrons of the transition metal sublattice [2, 4, 5]. The number of 3*d* electrons can be changed by the (transition metal/another transition metal) substitution. In the compound $Dy(Fe_{0.4}Co_{0.6})_2$, the majority 3*d* subband is completed and the minority 3*d* subband is filled up only partially. The transition metal sublattice behaves approximately like a strong ferromagnet [1].

In the present paper, the consequence of the Fe/Ni substitution, in the $Dy(Fe_{0.4}Co_{0.6})_2$ compound was studied. For this purpose, the synthesis, X-ray analysis and ^{57}Fe Mössbauer effect measurements were performed. The obtained results are qualitatively related to the Stoner model [7].

Crystal structure

The intermetallic compounds $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ (x = 0, 0.1, 0.2, 0.3) were prepared by arc melting in a high purity argon atmosphere from the appropriate amounts of Dy (99.9% purity), Fe, Co and Ni (all 99.999% purity).

The good quality X-ray patterns (Fig. 1) evidence the clean, cubic *Fd3m*, $MgCu_2$-type (C15) Laves phase across the series [2].

The determined lattice parameter a is presented in Table 1 and in Fig. 2. Since atomic radius of iron (r_{Fe} = 1.72 Å) is higher as compared to atomic radius of nickel (r_{Ni} = 1.62 Å), thus the lattice parameter $a(x)$ decreases

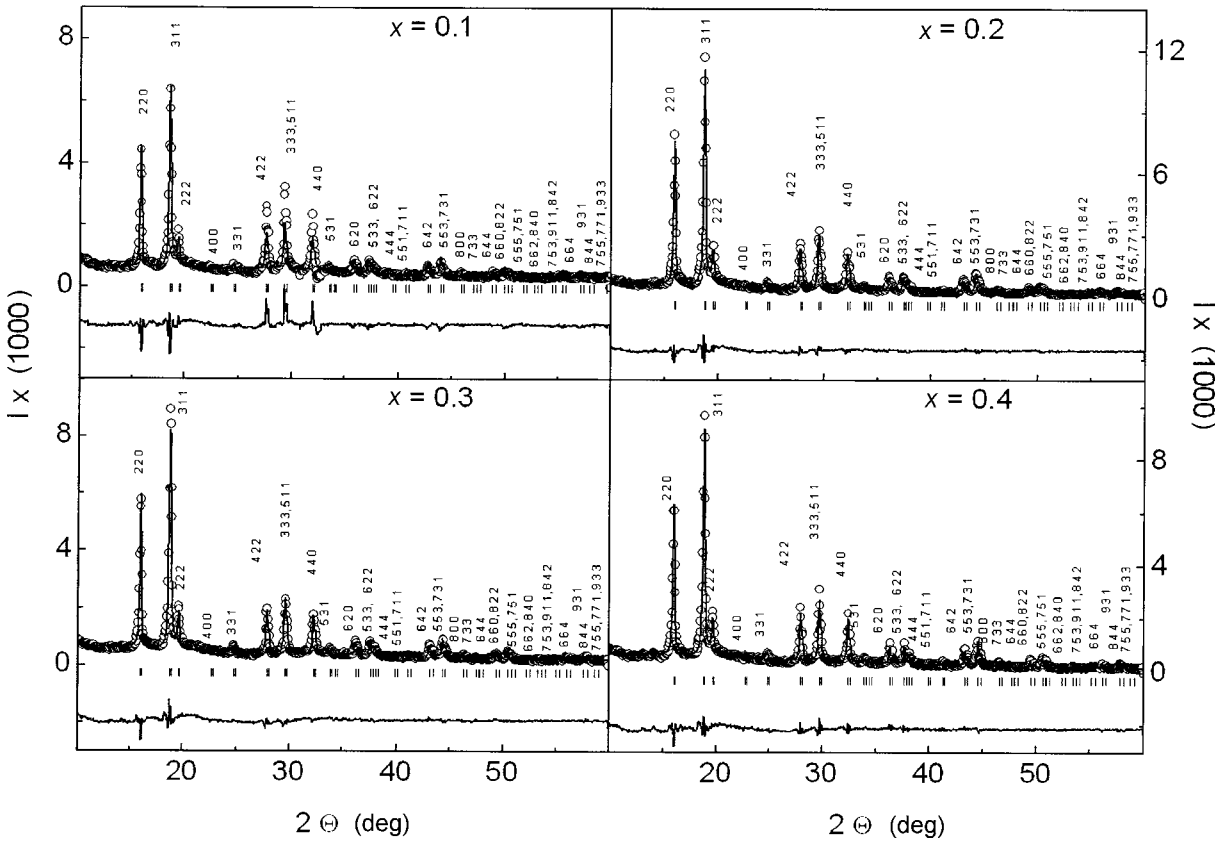

Fig. 1. X-ray patterns for $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ (295 K).

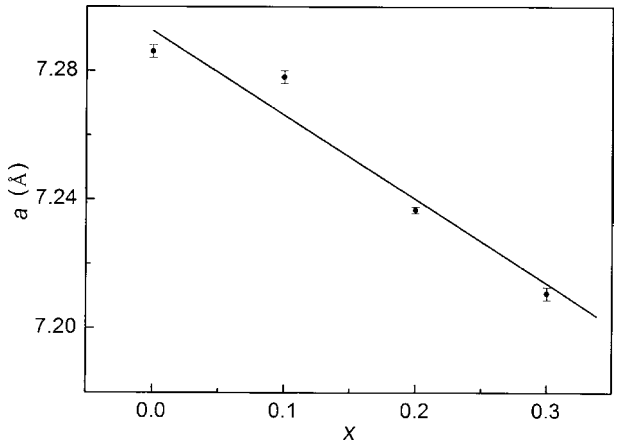

Fig. 2. Unit cell parameters for $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ ((•) – experimental points, (—) – fitted line $a(x)$ = (–0.262x + 7.292) Å).

with x. Experimental points of the crystal lattice parameters are described by a numerical equation: $a(x)$ = (–0.262x + 7.292) Å.

Mössbauer effect measurements

The Mössbauer effect measurements were performed at 77 K by using a standard transmission technique with a source of ^{57}Co in Rh.

The ^{57}Fe Mössbauer effect spectra observed for the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series are presented in Fig. 3. The analogous method to the used fitting procedure was described previously [5, 6]. As these spectra are composed of a number of subspectra, they are weakly resolved. This complexity should be mainly related to the different, presumably random (Fe, Ni, Co) nearest neighbour (n.n.) surroundings of the observed Fe atom resulting from the Fe/Ni substitution. Each (Fe, Ni, Co) n.n. surrounding introduces its own subspectrum and thus its own set of hyperfine interaction parameters. The n.n. surrounding is composed of n_1 Fe atoms, n_2 Ni atoms and n_3 Co atoms, with a crystal lattice condition for these numbers $n_1 + n_2 + n_3 = 6$. Assuming that the transition metal sublattice in the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ intermetallics is randomly populated by Fe, Ni and Co atoms with probabilities of $p_1 = 0.4 - x$, $p_2 = x$ and

Table 1. The crystal lattice and average hyperfine interaction parameters for $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$

x	n	a (Å)	IS (mm/s)	$\mu_0 H_{hf}$ (T)	QS (mm/s)
		295 K		77 K	
0	6.6	7.286(2)	0.014(8)	23.48(5)	0.057(8)
0.1	6.8	7.278(2)	0.019(26)	21.73(13)	0.060(26)
0.2	7.0	7.236(1)	0.019(17)	20.20(10)	0.058(17)
0.3	7.2	7.210(2)	0.027(32)	16.89(21)	0.073(32)

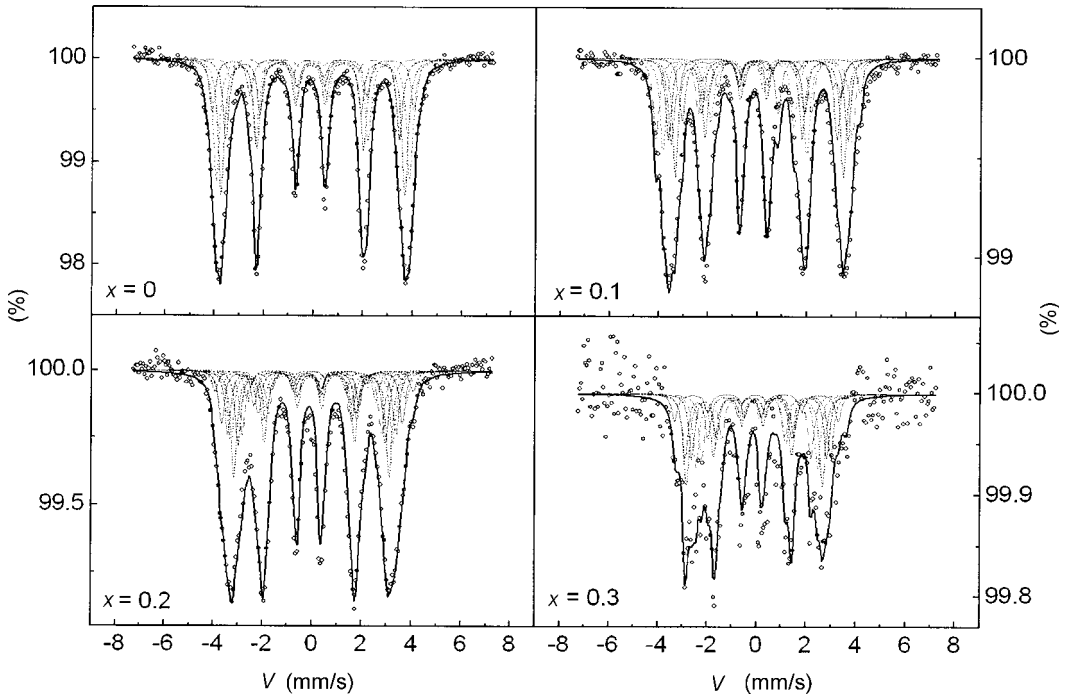

Fig. 3. ^{57}Fe Mössbauer effect transmission spectra of the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ intermetallics (77 K). Experimental points and fitted lines are presented.

$p_3 = 0.6$ ascribed to the Fe, Ni and Co atoms, respectively ($p_1 + p_2 + p_3 = 1$), the probabilities $P(\{6;n_1,n_2,n_3\})$ of the particular n.n. surroundings $\{6;n_1,n_2,n_3\}$ can be calculated using the general Bernoulli formula for intermediate compounds of the series, or using the ordinary Bernoulli formula for the borderline compounds of the series [3]. There is too big a number of different n.n. surroundigs $\{6;n_1,n_2,n_3\}$ and the corresponding probabilities $P(\{6;n_1,n_2,n_3\})$ to consider all of them during a fitting procedure. Therefore, a simplification should be made. Fortunately, there is a big group of vanishingly small probabilities which are calculated following the Bernoulli formulae. These can be omitted. The remaining probabilities we normalized again. During the fitting procedure it was asumed that the weights of subspectra follow these renormalized probabilities. A second quality Mössbauer spectrum and thus a second quality result of fitting procedure was obtained for the compound $Dy(Fe_{0.1}Ni_{0.3}Co_{0.6})_2$ due to a small content of iron. Table 1 and Fig. 4 contain the determined average hyperfine interaction parameters, i.e. the isomer shift IS (related to pure iron metal at 300 K), the magnetic hyperfine field $\mu_0 H_{hf}$ (μ_0 – magnetic permeability) and the quadrupole interaction parameter QS (as defined, for instance in [5, 6]).

Experimental points follow the fitted formulae: $IS(x) = 0.039x + 0.014$ mm/s, $\mu_0 H_{hf}(x) = -21.309x + 23.772$ T and $QS(x) = 0.046x + 0.055$ mm/s. The small values IS and QS increase slightly with x. The magnetic field $\mu_0 H_{hf}$ is strongly reduced across the series.

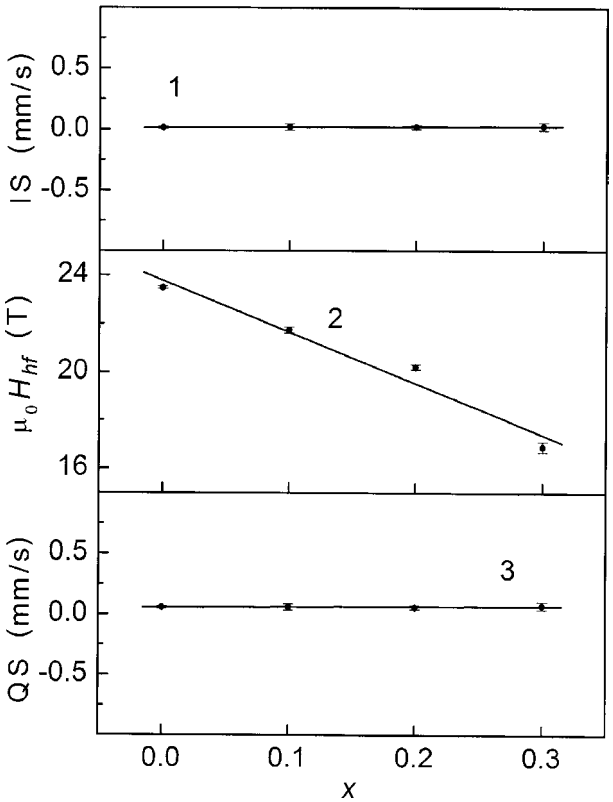

Fig. 4. Average hyperfine interaction parameters of the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series (77 K): 1 – the isomer shift IS in relation to Fe-metal, 295 K; 2 – the magnetic hyperfine field $\mu_0 H_{hf}$; 3 – the quadrupole interaction parameter QS.

The Slater-Pauling curve

The primary Slater-Pauling curve $\mu_0 H_{hf}$ obtained previously at 77 K for the series $Dy(Mn_{1-x}Fe_x)_2$ and $Dy(Fe_{1-x}Co_x)_2$ [4], is presented in Fig. 5 (line 1) for a comparison with the branch $\mu_0 H_{hf}(n)$ obtained for the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series (Fig. 5, line 2). In this case, the average number of 3*d* electrons calculated per one

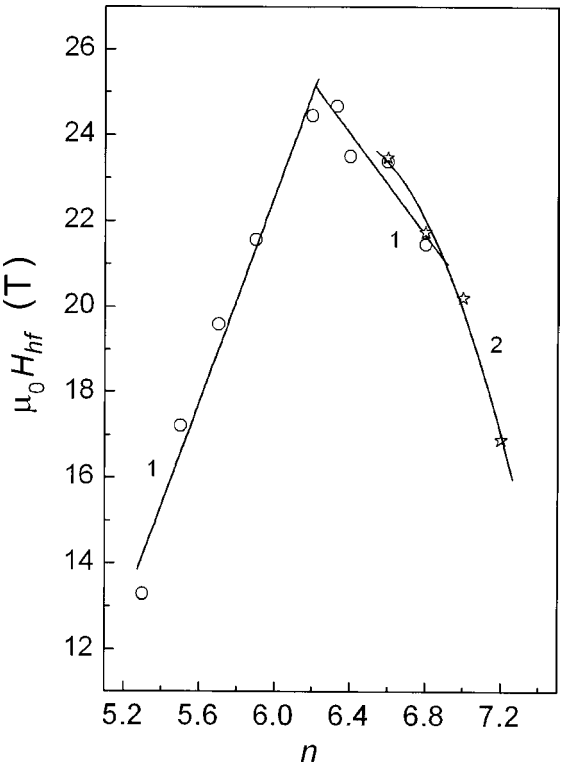

Fig. 5. Magnetic hyperfine fields $\mu_0 H_{hf}(n)$ (77 K) compared for series: 1 – experimental points (0) and fitted results for $Dy(Mn_{1-x}Fe_x)_2$ and $Dy(Fe_{1-x}Co_x)_2$ taken from [4]; 2 – experimental points (y) and fitted line $\mu_0 H_{hf}(n) = (-9.79n^2 + 124.49n - 371.69)$ T for $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$.

site of the transition metal sublattice can be expressed as $n(x) = (0.4 - x)\cdot 6 + 8x + 0.6\cdot 7$, where 6, 8 and 7 are numbers of 3*d* electrons of Fe, Ni and Co atoms respectively. The Fe/Ni substitution creates the $\mu_0 H_{hf}(n)$ branch which slightly bifurcates from the primary Slater-Pauling dependence. The experimental points are described by lines: 1 – $\mu_0 H_{hf}(n) = 12.01n - 49.46$ T and $\mu_0 H_{hf}(n) = -5.89n + 61.74$ T. The field of the new branch falls down nonlinearly with n. Line 2 is fitted using the formula $\mu_0 H_{hf}(n) = (-9.79n^2 + 124.49n - 371.69)$ T.

Discussion

The band structure of the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series is unknown as yet. Nevertheless, it has been found that the majority of 3*d*-subband of the starting $Dy(Fe_{0.4}Co_{0.6})_2$ compound of the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series is completed with 3*d* electrons and the minority 3*d* subband is filled up only partially [2]. In the series $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$, the substitution was used to introduce additional 3*d* electrons into the transition metal sublattice and thus to enforce changes in the 3*d* band. As a result, the $\mu_0 H_{hf}(n)$ field determined for the $Dy(Fe_{0.4-x}Ni_xCo_{0.6})_2$ series (Fig. 5, curve 2) can be treated as a certain continuation of the primary $\mu_0 H_{hf}(n)$ dependence. It seems that the Fe/Ni substitution should change the Fermi energy, the position of the 3*d* bands in relation to the Fermi level, the width of 3*d* bands and the energy shift between the 3*d* subbands [7]. In consequence of these changes, it is expected that the 3*d* electrons are gradually redistributed over the 3*d* subbands giving the observed $\mu_0 H_{hf}(n)$ dependence.

Since the 3*d* band properties are unknown as yet, at present a more detailed discussion is impossible. For a more precise discussion, the knowledge of band structure of the Fe/Ni-substituted intermetallic series would be helpful.

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