NUKLEONIKA 2004;49(Supplement 3):S85–S88

Mössbauer effect studies of $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ intermetallics

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

Abstract A consequence of the Fe/Ni substitution in the series of $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ was studied in the presented paper. The synthesis and X-ray analysis (300 K) of the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ system were performed. The cubic, $MgCu_2$-type, *Fd3m* crystal structure was evidenced for this solid solution. ^{57}Fe Mössbauer effect measurements for the system were carried out at 77 K. The obtained crystallographic lattice parameters and the hyperfine interaction data are presented. The magnetic hyperfine field values form a separate branch of the Slater-Pauling curve situated above the branch corresponding to the $Dy(Fe_{1-x}Co_x)_2$ intermetallics.

Key words intermetallics • crystal structure • ^{57}Fe Mössbauer effect • hyperfine interactions • Slater-Pauling curve • band structure

A. Jabłońska, J. Suwalski
Institute of Atomic Energy,
05-400 Otwock-Świerk, Poland

J. Pszczoła✉, P. Guzdek, P. Stoch
Solid State Physics Department,
AGH University of Science and Technology,
30 A. Mickiewicza Ave., 30-059 Kraków, Poland,
Tel.: +48 12/ 617 29 90, Fax: +48 12/ 634 12 47,
e-mail: pszczola@uci.agh.edu.pl

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

Received: 30 June 2004, Accepted: 10 August 2004

Introduction

^{57}Fe magnetic hyperfine fields $\mu_0 H_{hf}$ (μ_0 is the magnetic permeability), studied in the $Dy(Mn_{1-x}Fe_x)_2$ and $Dy(Fe_{1-x}Co_x)_2$ intermetallics, treated as a function of the average number n of 3d electrons per transition metal site, behave according to the Slater-Pauling type dependence [1].

Both the 3*d* subbands are filled-up across the $Dy(Mn_{1-x}Fe_x)_2$ series and the field $\mu_0 H_{hf}$ increases, but a completeness of the subbands is not reached. This tendency is continued across the $Dy(Fe_{1-x}Co_x)_2$ series and the majority of 3*d* subband is completed for the $Dy(Fe_{0.7}Co_{0.3})_2$ composition, the $\mu_0 H_{hf}$ field approaches its maximum. Further Fe/Co substitution populates only the minority 3*d* subband and reduces the $\mu_0 H_{hf}$ field. It was interesting to study the outcome of the Fe/Ni substitution in the $Dy(Fe_{0.7}Co_{0.3})_2$ compound (the Fe/Ni substitution introduces additional 3*d* electrons). For this purpose, the intermetallics $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ were synthesized and X-ray and ^{57}Fe Mössbauer effect studies were performed. Results are discussed within the frame of the rigid band model [3].

Experiment and results

The intermetallics $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ (x = 0, 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6) were prepared by arc melting. The cubic, *Fd3m*, $MgCu_2$-type (C15) Laves phase for the compounds was observed. The lattice parameters $a(x)$ are presented in Table 1.

The Mössbauer effect measurements were performed at 77 K and the spectra are presented in Fig. 1. The fitting procedure was analogous to a one described elsewhere [2].

Table 1. The crystal lattice parameters (295 K) and the average hyperfine interaction parameters (295 and 77 K) for $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$: n – average number of 3d electrons, IS – isomer shift, $\mu_0 H_{hf}$ – magnetic hyperfine field and QS – quadrupole interaction parameter.

x	a [Å]	n	$\mu_0 H_{hf}$ [T]	IS [mm/s]	QS [mm/s]
			295 K		
0.1	7.299(3)	6.5	21.38(12)	–0.116(16)	0.044(18)
0.2	7.287(3)	6.7	19.80(15)	–0.140(19)	0.061(23)
0.3	7.271(3)	6.9	16.71(9)	–0.116(14)	0.029(16)
0.4	7.241(3)	7.1	12.21(6)	–0.074(9)	0.118(9)
0.5	7.216(3)	7.3	–	–0.025(15)	0.311(28)
0.6	7.194(3)	7.5	–	–0.089(22)	0.252(224)
			77 K		
0.1	–	6.5	23.95(12)	0.024(17)	0.038(18)
0.2	–	6.7	23.12(9)	–0.082(25)	0.052(27)
0.3	–	6.9	21.80(6)	0.020(8)	0.048(10)
0.4	–	7.1	20.29(6)	0.019(8)	0.048(10)
0.5	–	7.3	18.42(7)	0.023(11)	0.058(12)
0.6	–	7.5	14.77(22)	0.019(23)	0.072(34)

The average values of the hyperfine interaction parameters, i.e., the isomer shift IS (with respect to pure iron metal at 300 K), the magnetic hyperfine field $\mu_0 H_{hf}$ and the quadrupole interaction parameter QS determined for the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series are presented in Fig. 2. Additionally, the parameters are listed in Table 1. The average parameters are described by the numerical formulas: $IS(x) = [0.021(8)x + 0.002(30)]$mm/s, $\mu_0 H_{hf}(x) = [-23.91(4.05)x^2$

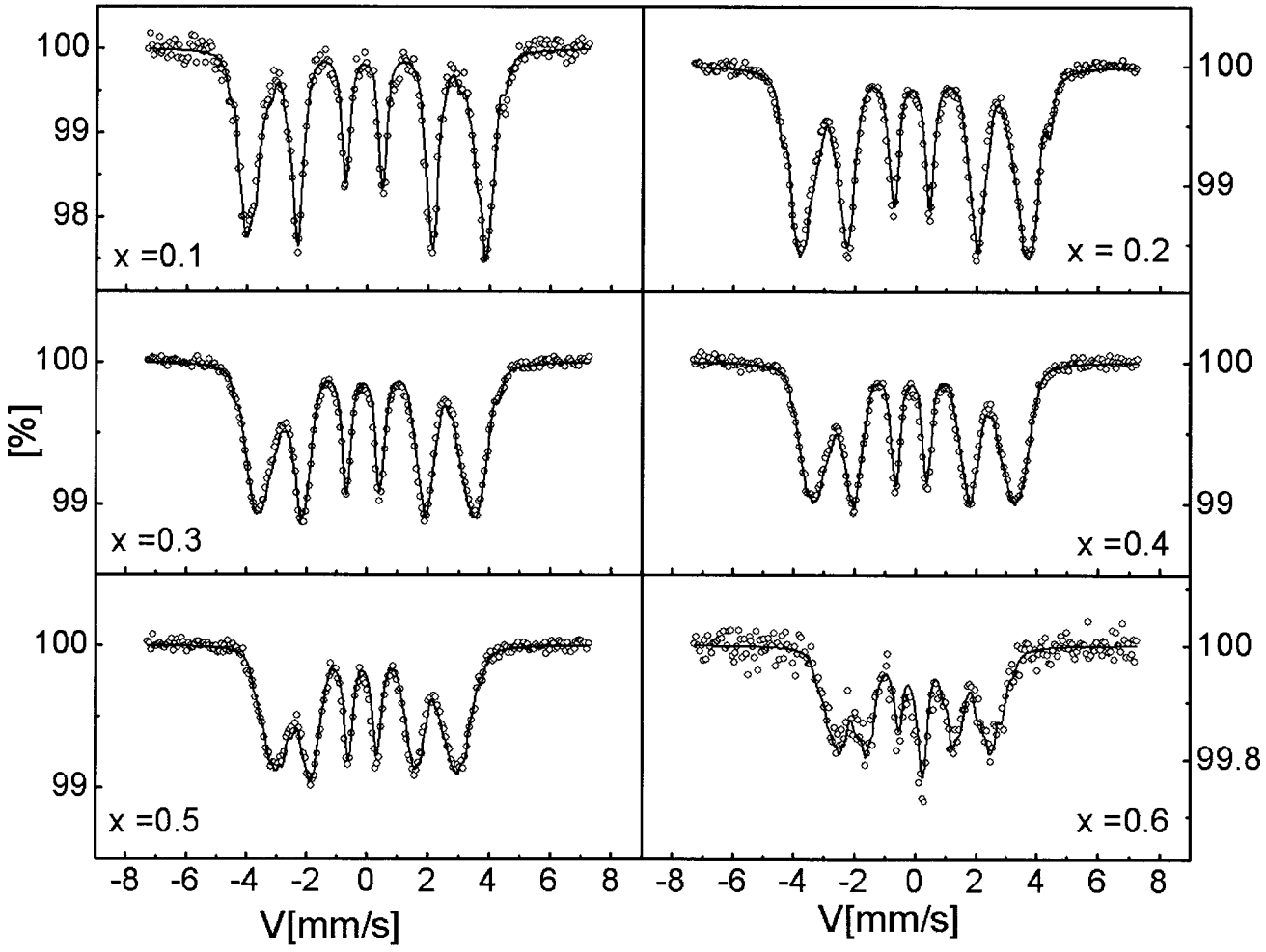

Fig. 1. ^{57}Fe Mössbauer effect transmission spectra of the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ intermetallics (77 K). Experimental points and fitted lines are presented.

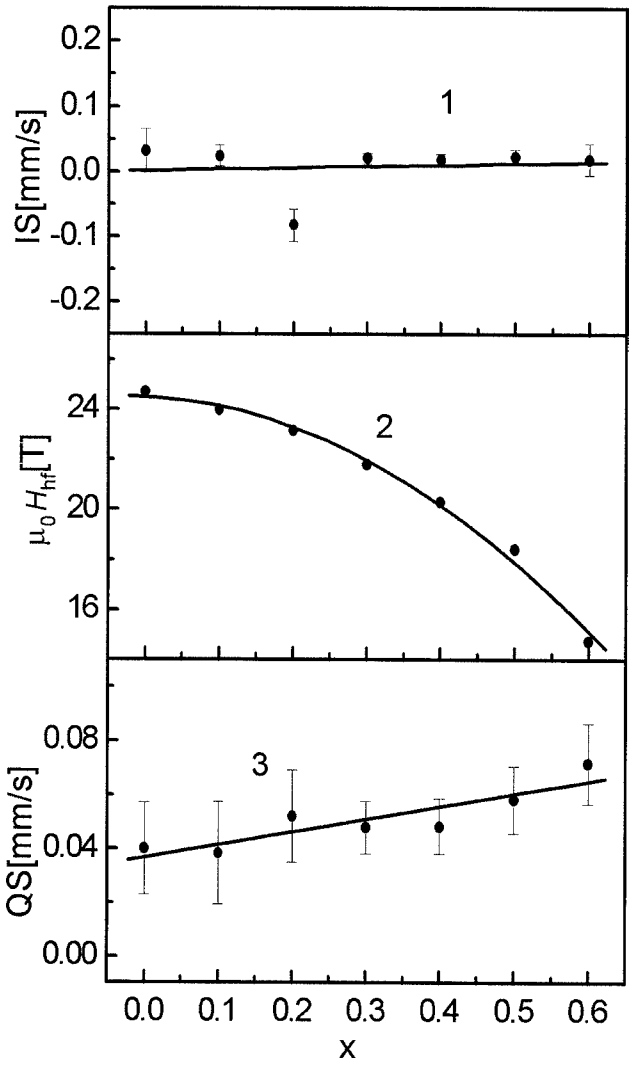

Fig. 2. Average hyperfine interaction parameters of the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series (77 K): 1 – the isomer shift IS in relation to Fe-metal, 300 K; 2 – the magnetic hyperfine field $\mu_0 H_{hf}$; 3 – the quadrupole interaction parameter QS.

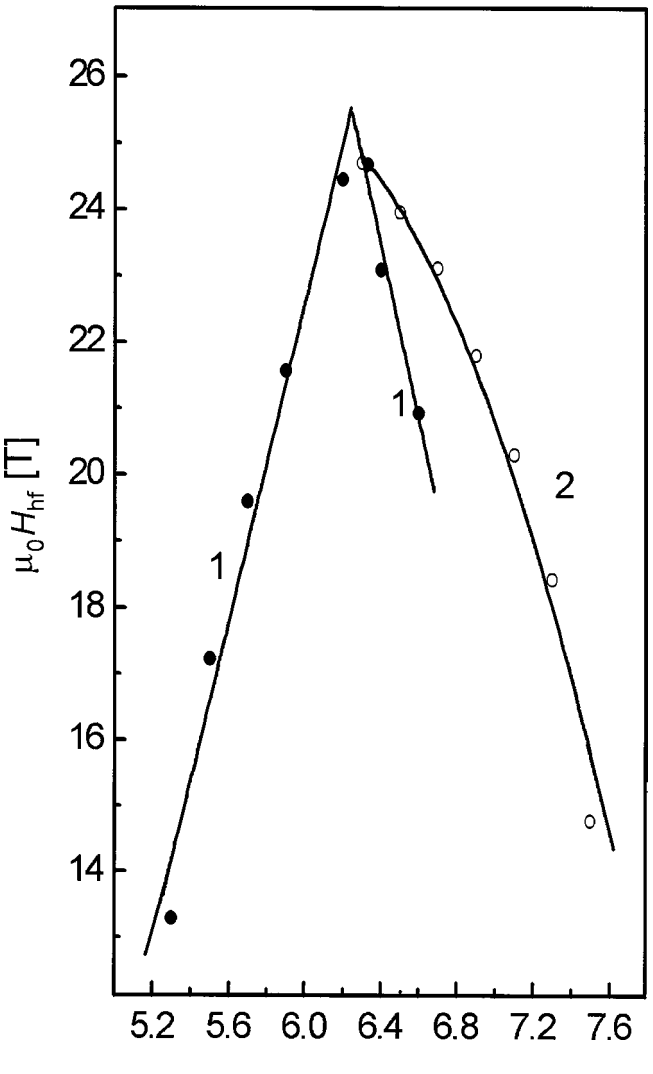

Fig. 3. Magnetic hyperfine fields $\mu_0 H_{hf}(n)$ (77 K) compared for series: 1 – $Dy(Mn_{1-x}Fe_x)_2$, $Dy(Fe_{1-x}Co_x)_2$ and 2 – $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$.

– 1.24(2.53)x + 24.48(0.32)]T and QS(x) = [0.047(10)x + 0.037(4)]mm/s.

The Slater-Pauling curve

The Slater-Pauling curve $\mu_0 H_{hf}(n)$, obtained previously for the series $Dy(Mn_{1-x}Fe_x)_2$ and $Dy(Fe_{1-x}Co_x)_2$ [1], is presented in Fig. 3 (line 1) for a comparison with the branch $\mu_0 H_{hf}(n)$ obtained for the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series (Fig. 3, line 2). In this case, the average number of 3d electrons calculated per one site of the transition metal sublattice can be expressed as $n(x) = (0.7 - x)^*6 + 8x + 0.3^*7$, where 6, 8 and 7 are numbers of 3d electrons of Fe, Ni and Co atoms, respectively. The Fe/Ni substitution creates the $\mu_0 H_{hf}(n)$ branch which bifurcates from the top area of the Slater-Pauling dependence. The experimental points are described by lines: $1 - \mu_0 H_{hf}(n)$ = [12.0(1.1)n – 49.4(6.5)]T, $1 - \mu_0 H_{hf}(n)$ = [–13.2(2.4)n + 108.0(16.5)]T. The field of this new branch falls down nonlinearly with increasing n. Line 2 is fitted using the formula $\mu_0 H_{hf}(n)$ = [–3.5(1.0)n^2 + 40.7(27.0)n – 92.9(10.1)]T.

Summary and discussion

The band structure of the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series is unknown as yet. Nevertheless, it has been found that the majority of 3d-subband of the starting compound $Dy(Fe_{0.7}Co_{0.3})_2$ of the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series is completed with 3d electrons and the magnetic hyperfine field $\mu_0 H_{hf}$ approaches its maximal value [1]. In the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series, the Fe/Ni substitution was used to introduce additional 3d electrons into the transition metal sublattice and thus to enforce changes in the 3d band. As a result, the determined $\mu_0 H_{hf}(n)$ dependence for the $Dy(Fe_{0.7-x}Ni_xCo_{0.3})_2$ series (Fig. 3, curve 2) is situated above the $\mu_0 H_{hf}(n)$ dependence corresponding for the rest (x > 0.3) of the $Dy(Fe_{1-x}Co_x)_2$ series. It seems that the Fe/Ni substitution should change the Fermi energy, the position of the 3d bands in relation to the Fermi level, the width of 3d bands and the energy shift between 3d subbands [3]. In consequence of these changes, it is expected that the 3d electrons are gradually and adequately redistributed over the 3d subbands giving the observed $\mu_0 H_{hf}(n)$ dependence.

Since the 3d 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 is necessary.

Acknowledgment Supported partially by the State Committee for Scientific Research, grant No. 3T08D04827. M. Mróz and T. Winek are acknowledged for technical assistance.

References

1. Gicala B, Pszczoła J, Kucharski Z, Suwalski J (1995) Magnetic hyperfine fields of $Dy_x(Fe\text{-}Co)_y$ compounds. Solid State Commun 96:511–515
2. Stoch P, Pszczoła J, Jagodziński P *et al*. (2004) Synthesis, crystal structure and Mössbauer effect studies of $Dy(Mn_{0.4}Fe_{0.6-x}Al_x)_2$ intermetallics. J Alloys Compd 375:24–30
3. Vonsovskij W (1971) Magnetizm. Nauka, Moscow (in Russian)