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Crystal structure and Mössbauer effect studies of $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ intermetallics

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Abstract. X-ray crystal structure (300 K) and ^{57}Fe Mössbauer effect (77 K) studies were performed for the $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ compounds. The crystal lattice parameter decreases vs. an average number of 3*d* electrons. The magnetic hyperfine field treated as a function of the average number of 3*d* electrons forms a Slater-Pauling type dependence. This dependence is related to the 3*d*-electron band structure within the frame of the rigid band model.

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

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Introduction

Fundamental interest and practical applications are the reason behind the numerous studies of the heavy rare earth (R) – transition metal (M) compounds [1, 2, 6, 7]. It was previously found that the hyperfine interactions and the magnetic properties of the R-M materials are mainly governed by the 3*d* electrons of the M sublattice [3, 5].

Thus, it was interesting to study the significance of the Mn/Fe and Fe/Co substitution in the $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ intermetallics. For this purpose, crystal structure and ^{57}Fe Mössbauer effect studies were performed. The obtained data are qualitatively discussed within the frame of the rigid band model [8].

Experiment

The intermetallics $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ ($0 \le x \le 1$) were prepared by arc melting, in a high purity argon atmosphere from the appropriate amounts of Gd (99.9% purity), Mn, Fe and Co (all 99.99% purity).

From the X-ray patterns, the cubic, *Fd*3*m*, $MgCu_2$-type (C15) Laves phases were deduced for all the compounds. Since the atomic radius is reduced across the transition metal series (r_{Mn} = 1.79 Å, r_{Fe} = 1.72 Å and r_{Co} = 1.67 Å) thus the lattice parameter $a(n)$ (Fig. 1) is reduced vs. the average number n of 3*d* electrons calculated per transition metal atom. A typical deviation for R-M intermetallics from Vegard's rule is observed also for studied compounds. Line in Fig. 1 following experimental points is described by a numerical formula $a(n) = (-0.109n^3 + 2.062n^2 - 13.123n + 35.440)$ Å.

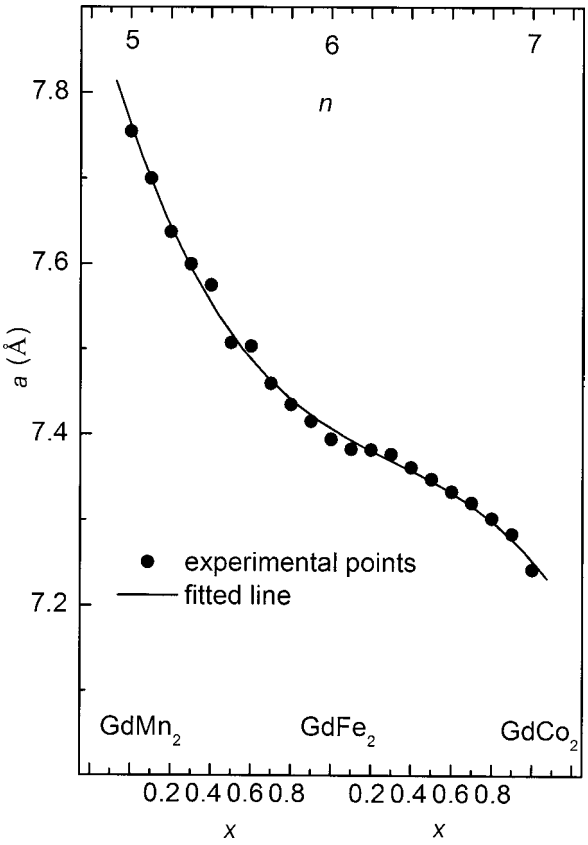

Fig. 1. The crystal lattice parameters of the $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ compounds (300 K) vs. n the average number of 3*d* electrons.

Mössbauer spectra were collected using a standard transmission technique with a Co/Rh source. The resulting ^{57}Fe Mössbauer effect spectra (at 77 K) for the $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ series are presented in Figs. 2 and 3, respectively. Fitting procedure was performed considering both the <111> easy axis of magnetization (two subspectra with the ratio 0.25/0.75) and the assumed random distribution of transition metal atoms (Bernoulli distribution) by an analogous method as presented previously elsewhere [4]. Figure 4 contains the determined average hyperfine

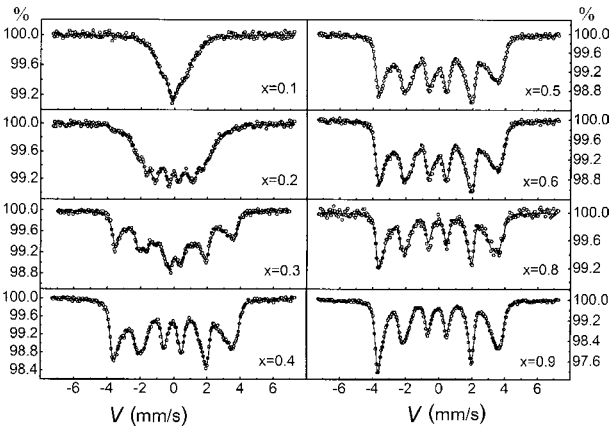

Fig. 2. ^{57}Fe Mössbauer effect spectra of the $Gd(Mn_{1-x}Fe_x)_2$ intermetallics (77 K). Experimental points and fitted lines are presented.

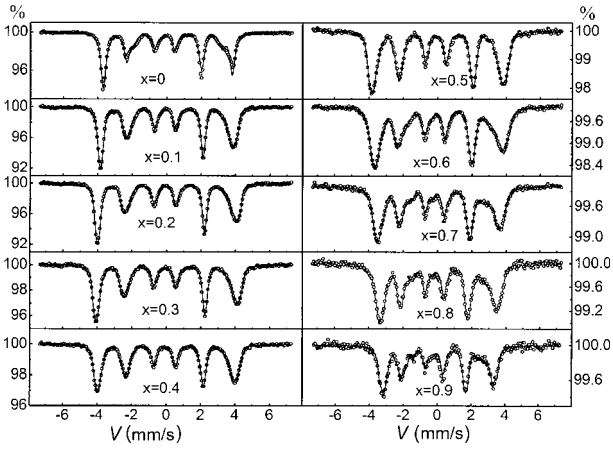

Fig. 3. ^{57}Fe Mössbauer effect spectra of the $Gd(Fe_{1-x}Co_x)_2$ intermetallics (77 K). Experimental points and fitted lines are presented.

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 is the magnetic permeability) and the quadrupole interaction parameter QS (as defined for instance in [6]). The dependencies (1, 4, 5) and (2, 3, 6) correspond to the 0.25 and the 0.75 subspectra, respectively. As a result of considerable experimental errors, as compared to small IS and QS values lines 1, 2 and 5, 6 are weakly resolved. Nevertheless, curves 3 and 4 are resolved satisfactorily. Both these curves follow a Slater-Pauling type dependence.

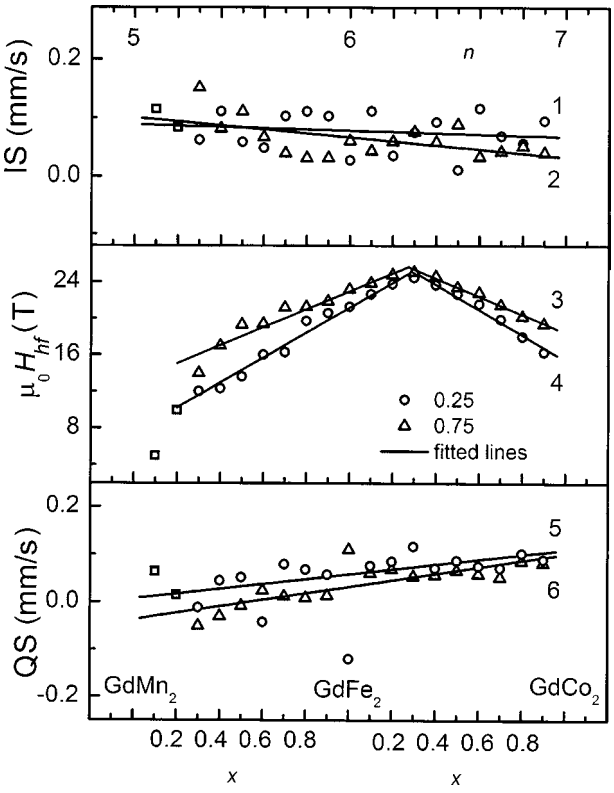

Fig. 4. Average hyperfine interaction parameters of the $Gd(Mn_{1-x}Fe_x)_2$ and $Gd(Fe_{1-x}Co_x)_2$ series (77 K): (1, 4, 5) and (2, 3, 6) the hyperfine interaction parameters for the 0.25 and the 0.75 subspectra, respectively.

Discussion

The substitution of one transition metal by another transition metal strongly influences the magnetic hyperfine fields. As a result of the Mn/Fe and Fe/Co substitution, the field $\mu_0 H_{hf}(n)$ creates the Slater-Pauling type curve. At first, the strong ferromagnetism-type behavior of the M-sublattice is observed. The magnetic hyperfine field in the $Gd(Mn_{1-x}Fe_x)_2$ series grows up with x. This growth occurs for the $Gd(Fe_{1-x}Co_x)_2$ series too, and the maximum value of the field is approached for the $Gd(Fe_{0.7}Co_{0.3})_2$ compound (at $x = 0.3$, $n = 6.3$). At this Co-content, the filling up of the majority 3*d*-subband by 3*d*-electrons is terminated. For the higher Co-substitutions, the weak ferromagnetism-type behavior of the M-sublattice appears. The filling up of the minority 3*d*-subband still proceeds, and the observed field decreases gradually with n. The $\mu_0 H_{hf}$ field strongly depends on the average number n of 3*d* electrons calculated per transition metal atom.

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