Mössbauer effect studies of Dy(Mn_{0.4−x}Al_{x}Fe_{0.6})₂ compounds

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Abstract

It was previously found that the magnetic hyperfine fields observed at ⁵⁷Fe nuclei (4.2 K) in the Dy(Mn_{1−x}Fe_{x})₂ and Dy(Fe_{1−x}Co_{x})₂ intermetallics form a Slater–Pauling curve. Both 3d subbands in the Dy(Mn_{0.4}Fe_{0.6})₂ compound are filled up only partially with 3d electrons.

The consequence of Mn/Al substitution, in the Dy(Mn_{0.4}Fe_{0.6})₂ compound was studied in the present paper. For this purpose the synthesis and X-ray analysis (300 K) of the series Dy(Mn_{0.4−x}Al_{x}Fe_{0.6})₂ were performed. The cubic, MgCu₂-type Fd3m crystal structure was observed across the series. Nevertheless for x = 0.35 and 0.40 a stoichiometric admixture of the hexagonal, MgZn₂-type, P6₃/mmc was evidenced.

⁵⁷Fe Mössbauer effect measurements for the series were performed at 4.2 K. The magnetic hyperfine fields form a separate branch of the Slater–Pauling curve. This branch is compared to the magnetic hyperfine field previously obtained for the Dy(Mn_{0.4}Fe_{0.6−x}Al_{x})₂ series (the Fe/Al substitution). The possible 3d electron band structure is discussed qualitatively within the Stoner model.

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Keywords: Intermetallics; Crystal structure; ⁵⁷Fe Mössbauer effect; Hyperfine interactions; Slater–Pauling curve; Band structure

1. Introduction

Fundamental interest and practical applications are the reason behind the numerous studies of the heavy rare earth (R)-transition metal (M) compounds [1–3]. The ferrimagnetism of the R–M compounds results from the coexistence between the 4f (5d) and 3d electron magnetism [4–6]. It was previously found that the magnetic properties of the R-M materials are mainly governed by the 3d electrons of the transition metal sublattice [4–6]. However, the electronic band structure of the R-M intermetallics, especially of their transition metal constituent, is rather complex and poorly known up to date.

Systematic Mössbauer effect studies of the substituted RM₂ series of compounds were a useful method to test both the rare earth and the transition metal sublattice and thus to clarify the 3d-5d-4f magnetism [5]. In particular, it was previously found that the magnetic hyperfine field \( \mu_0 H_{hf} \) (\( \mu_0 \) is the magnetic permeability), determined at \( ^{57}\text{Fe} \) nuclei in the Dy(Mn_{1−x}Fe_{x})₂ and Dy(Fe_{1−x}Co_{x})₂ intermetallic series, treated as a function of the average number \( n \) of 3d electrons calculated per transition metal site (in analogy to the 3d metal–3d metal alloys [7–9]) behave according to the Slater–Pauling curve with a maximum hyperfine field appearing for the Dy(Fe_{0.7}Co_{0.3})₂ compound [5,6].

Across the Dy(Mn_{1−x}Fe_{x})₂ series the 3d subbands are filled up step by step and consequently the magnetic hyperfine field \( \mu_0 H_{hf} \) increases with \( x \) (or \( n \)) [5]. It can be noticed that in this series no one 3d subband approaches its completeness.

Al substitution is a widely used method to modify 3d bands and thus to modify the magnetic properties and hyperfine interactions, as for instance in Refs. [10,11]. Al atom substituted into the M sublattice introduces the 3s²3p¹ electrons instead of the 3d⁶4s² electrons of manganese atom. This replacing strongly influences the 3d band and thus the magnetism and hyperfine interactions of the compounds [10–15].

The significance of the iron component was studied recently using Fe/Al substitution in the series Dy(Mn_{0.4}Fe_{0.6−x}Al_{x})₂ (the 3d subbands are populated only partially) [16].
It would be interesting to study, for a comparison, the significance of the manganese component in the compounds, with the 3d subbands only partially occupied by 3d electrons. Thus to test the influence of the manganese atoms on the 4f–5d–3d magnetism and especially on the magnetism of the 3d sublattice, Mn/Al substitution in the Dy(3d$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ series was used in the present paper. The compounds Dy(3d$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ were synthesized and subsequently X-ray and $^{57}$Fe Mössbauer effect measurements were performed. The obtained data are qualitatively discussed within the frame of the rigid band model.[9,17,18]

**2. Materials and crystal structure**

New intermetallics Dy(3d$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ ($x = 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35 and 0.40) were prepared by arc melting, in a high-purity argon atmosphere from the appropriate amounts of Dy (99.9% purity), Mn, Fe and Al (all 99.99% purity) as starting materials.

The X-ray patterns obtained for these compounds (Fig. 1) were analyzed using the Rietveld-type procedure [19,20]. The cubic, Fd3m, MgCu$_2$-type (C15) Laves phases [21–23] were observed across the series. Nevertheless, for $x = 0.35$ and 0.40 an admixture (presumably stoichiometric) of the

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**Fig. 1.** X-ray powder diffraction patterns observed for the Dy(3d$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ intermetallics (300 K) in the mixed region. Asterisk denotes the second crystallographic phase in the mixed region. Fitted differential pattern is added below each diffractogram.

**Fig. 2.** The crystal lattice parameters of the Dy(3d$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ intermetallics (300 K) in the MgCu$_2$-type structure: (1) the lattice edge $a$, (2) the unit cell volume $V$ and (3) the volume $w$ calculated per atom.
hexagonal, P63/mmc, MgZn2-type (C14) Laves phase can be observed. A possible coexistence of the stoichiometric similar C14 and C15 Laves phases in the compound was previously discussed elsewhere[24].

For further practical reasons, it is worth noticing that the MgCu2-type unit cell contains eight stoichiometric formula units, i.e. 24 atoms: 8 Mg and 16 Cu atoms. Each Cu (or transition metal atom M) has six Cu (or M) atoms in the nearest neighbor shell (radius: \(a(2)/2/4\)) [21,22].

The lattice parameters \(a\) and \(c\) obtained from the fitting procedure, the unit cell volume \(V\) and the volume \(w\) per atom are presented in Table 1 (the value at \(x = 0\) estimated from data of the Dy(Mn1−xAlxFex)2 series [25] and the value for \(x = 0.4\) are added [13]). Moreover the \(a\), \(V\) and \(w\) data for the MgCu2-type of structure are presented in Fig. 2. In practice the Vegard rule is obeyed and thus a linear dependence for the \(a(x)\) parameter, described by the numerical formula \(a(x) = [0.352(13)x + 7.393(3)]\AA\), is observed.

### Table 1

Crystallographic data for the Dy(Mn0.4−xAlxFe0.6)2 series (300 K).

<table>
<thead>
<tr>
<th>(x)</th>
<th>Phase (%)</th>
<th>(a) (Å)</th>
<th>(c) (Å)</th>
<th>(V) (Å³)</th>
<th>(w) (Å³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>MgCu2-type phase</td>
<td>0.35</td>
<td>100</td>
<td>7.39(1); 7.37(2) [25]</td>
<td>403.7(5)</td>
</tr>
<tr>
<td>0.05</td>
<td>MgCu2-type phase</td>
<td>0.4</td>
<td>100</td>
<td>7.40(1)</td>
<td>406(7(2)</td>
</tr>
<tr>
<td>0.10</td>
<td>MgCu2-type phase</td>
<td>0.4</td>
<td>100</td>
<td>7.43(1)</td>
<td>410.7(2)</td>
</tr>
<tr>
<td>0.15</td>
<td>MgCu2-type phase</td>
<td>0.5</td>
<td>100</td>
<td>7.446(1)</td>
<td>412.8(1)</td>
</tr>
<tr>
<td>0.20</td>
<td>MgCu2-type phase</td>
<td>0.5</td>
<td>100</td>
<td>7.4649(8)</td>
<td>416.0(1)</td>
</tr>
<tr>
<td>0.25</td>
<td>MgCu2-type phase</td>
<td>0.6</td>
<td>100</td>
<td>7.4793(9)</td>
<td>418.4(2)</td>
</tr>
<tr>
<td>0.30</td>
<td>MgCu2-type phase</td>
<td>0.6</td>
<td>58(2)</td>
<td>7.502(1)</td>
<td>422.2(2)</td>
</tr>
<tr>
<td>0.35</td>
<td>MgCu2-type phase</td>
<td>0.6</td>
<td>58(2)</td>
<td>7.509(3)</td>
<td>423.4(5)</td>
</tr>
<tr>
<td>0.40</td>
<td>MgCu2-type phase</td>
<td>0.6</td>
<td>58(2)</td>
<td>7.560(1)</td>
<td>432(2)</td>
</tr>
<tr>
<td>0.35</td>
<td>MgZn2-type phase</td>
<td>0.35</td>
<td>100</td>
<td>5.328(1)</td>
<td>8.630(1)</td>
</tr>
<tr>
<td>0.4</td>
<td>MgZn2-type phase</td>
<td>0.4</td>
<td>68(3)</td>
<td>5.319(1); 5.319(3) [13]</td>
<td>8.683(1); 8.686(2)</td>
</tr>
</tbody>
</table>

\(a\), \(c\): unit cell parameters; \(V\): unit cell volume; \(w\): volume per atom.

### 3. Spectra and analysis

The Mössbauer effect measurements were performed at 4.2 K by using a standard transmission technique with a source of \(^{57}\)Co in Rh.

The experimental \(^{57}\)Fe Mössbauer effect spectra (points) observed for the Dy(Mn0.4−xAlxFe0.6)2 series (\(x = 0, 0.05, 0.10, 0.15, 0.20\) and \(0.30\)) are presented in Fig. 3. 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 \([\text{Mn, Al, Fe}]\) nearest neighbor (n.n.) surroundings of the observed Fe atom resulting from the Mn/Al substitution. Each \([\text{Mn, Al, Fe}]\) n.n. surrounding introduces its own subspectrum and thus its own set of hyperfine interaction parameters. Following formula \(\text{Dy}(\text{Mn}0.4\text{Al}_{0.6})\text{Fe}_{x}\) it can be noticed that there are probabilities \(p_1 = (0.4 - x), p_2 = x\) and \(p_3 = 0.6\) to find in the crystal lattice the Mn, Al and Fe atom, respectively.

![Fig. 3. \(^{57}\)Fe Mössbauer effect transmission spectra of the Dy(Mn0.4−xAlxFe0.6)2 intermetallics (4.2 K). Experimental points, fitted lines and fitted subspectra are presented.](image-url)
The fitting procedure of the spectra was carried out analogously as for the series Dy(Mn\(_{0}\),Al\(_{0}\),Fe\(_{x}\))\(_{2}\) described previously [16]. The fitted subspectra and the resulting fitted spectrum (lines) are presented in Fig. 3 for each compound of the series studied by Mössbauer effect.

It can be added that the n.n. surrounding is composed of \(n_{1}\) Mn atoms, \(n_{2}\) Al atoms and \(n_{3}\) Fe atoms. The probabilities \(P(\{0,1,2,3\})\) of the particular n.n. surroundings were calculated using the Bernoulli formulae [26]. As mentioned above \(l = 6\) is the number of n.n. in the transition metal sublattice surrounding the studied Fe atom. Although the number of the probabilities \(P(\{0,1,2,3\})\) is quite large, there is a considerable number of the vanishingly small probabilities and these can be neglected during the fitting procedure.

Exemplary fitting results for the compound Dy(Mn\(_{0}\),Al\(_{0}\),Fe\(_{x}\))\(_{2}\) are presented in Table 2. As in the case of the Dy(Mn\(_{0}\),Fe\(_{x}\))\(_{2}\) series it was assumed that the magnetically most important constituents are the Fe atoms [16]. In the table there is presented the probability \(P(\{0,1,2,3\})\) follow the probabilities \(P(i)\). Since in the series Dy(Mn\(_{0}\),Al\(_{0}\),Fe\(_{x}\))\(_{2}\) the probability to find an Fe atom in the crystal lattice is constant \((p_{3} = 0.6)\), the distributions of probabilities \(P(i)\) are the same across the series (Fig. 4), within the frame of the used approximation (neglected small probabilities) [26]. The calculated probabilities \(P(\{0,1,2,3\})\) and the fitted weights \(W(\{0,1,2,3\})\) are contained in Table 2. First of all, the table contains the determined hyperfine interaction parameters, i.e. the isomer shift \(\mu_{IS}\) (related to pure iron metal at 300 K), the magnetic hyperfine field \(\mu_{H}\) and the quadrupole interaction parameter \(\Delta\) (defined in Ref. [27]) and their average values calculated following the formula \(X = \sum_{i=1}^{n} W(i)X_{i}/\sum_{i=1}^{n} W(i)\). Actually, it is impossible during the numerical analysis to consider all the factors reflecting the physical complexity of the problem. For instance, the influence of the next nearest neighbor configurations, and a possible deviation from randomness among atoms were not taken into account and thus some arbitrariness of the fitting procedure cannot be avoided. Consequently, some differences between \(P\) (open rectangles) and \(W\) (shaded rectangles) are observed (Fig. 4).

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Nevertheless, taking into account the mentioned complexity of the spectra and thus of the fitting procedure, the probabilities \(P\) and the weights \(W\) seem to be satisfactorily similar.
4. Average hyperfine interaction parameters

The determined average values of the hyperfine interaction parameters of the Dy(Mn$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ compounds are presented in Fig. 5. Moreover, the values of the parameters are listed in Table 3. Additionally, the previous literature data for $x = 0$ and $x = 0.4$ are included in the figure and the table [13,25].

The average isomer shift $IS(x)$ equals 0.070(5) mm/s at $x = 0$, increases linearly across the series Dy(Mn$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ and approaches the value 0.148(5) mm/s at $x = 0.3$. Experimental points follow the fitted formula $IS(x) = [0.218(27)x + 0.078(6)]$ mm/s. Considering this formula the extrapolated value of IS, 0.178 mm/s for $x = 0.4$, can be found. This value is relatively close to the IS parameter [=0.154(29) mm/s] known for Dy(Al$_{0.4}$Fe$_{0.6}$)$_2$ [13].

The mechanism responsible for the change in isomer shift was already discussed in detail elsewhere [10].

The magnetic hyperfine field $\mu_0H_{hf}$ equals 17.34(5) T for Dy(Mn$_{0.4}$Fe$_{0.6}$)$_2$ (this value fits well to the dependence $\mu_0H_{hf}(n)$ observed for the Dy(Mn$_{1-y}$Fe$_y$)$_2$ series [6,25]) and decreases considerably with the Al content $x$ to the value 13.1(5) T for $x = 0.3$ and 12.98(7) T for $x = 0.4$ [13]. The line through the experimental points corresponds to a linear fit: $\mu_0H_{hf}(x) = [-10.82(95)x + 16.72(28)]$ T.

The quadrupole interaction parameter QS adopts small values and it is expected that it slightly increases with $x$, if it varies at all.

5. The branch of the Slater–Pauling curve

The 3d/3d Slater–Pauling curve $\mu_0H_{hf}(n)$, a result of the substitution of one transition metal by the other, observed for the Dy(M–M)$_2$ compounds (M–M = Mn–Fe, Fe–Co) [5,6] (Fig. 6, line 1; $\mu_0H_{hf} = 12.03(5)\text{n} - 49.23\text{[2.971]}$, $\mu_0H_{hf} = [-4.14(1.05)\text{n} + 51.68(6.741)]$ T), and the $\mu_0H_{hf}(n)$ data of the Dy(Mn$_{0.4}$Fe$_{0.6}$)$_2$ series [16] (Fig. 6, line 2; $\mu_0H_{hf} = [0.957(268)\text{n} - 4.086(2.369)\text{n} + 10.366(5.074)]$ T) are compared with the $\mu_0H_{hf}(n)$ branch (Fig. 6, line 3; $\mu_0H_{hf} = [1.196(63)\text{n}^2 - 5.982(1.438)\text{n} - 14.044(3.081)]$ T) obtained for the Dy(Mn$_{0.4-x}$Al$_x$Fe$_{0.6}$)$_2$ series. In the last case, the average number of 3d electrons...
Fig. 6. Magnetic hyperfine fields \( \mu H_{hf}(n) \) (4.2 K) compared for series (1) Dy(Mn\(_{6-x}\),Al\(_x\)Fe\(_{6-y}\)), (2) Dy(Mn\(_{6-x}\),Al\(_x\)Fe\(_{6-y}\)), and (3) Dy(Mn\(_{6-x}\),Al\(_x\)).

<table>
<thead>
<tr>
<th>( x )</th>
<th>( n )</th>
<th>( G ) (mm/s)</th>
<th>IS (mm/s)</th>
<th>( \mu H_{hf} ) (T)</th>
<th>QS (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.160</td>
<td>0.171</td>
<td>0.070(5)</td>
<td>0.042(50)</td>
<td>17.340(5) 18.40(8)</td>
</tr>
<tr>
<td>0.1</td>
<td>0.160</td>
<td>0.171</td>
<td>0.087(6)</td>
<td>0.130(5)</td>
<td>16.13(7) 0.020(4)</td>
</tr>
<tr>
<td>0.15</td>
<td>0.160</td>
<td>0.170</td>
<td>0.096(5)</td>
<td>13.74(5)</td>
<td>0.016(3)</td>
</tr>
<tr>
<td>0.2</td>
<td>0.170</td>
<td>0.170</td>
<td>0.136(8)</td>
<td>14.29(5)</td>
<td>0.018(4)</td>
</tr>
<tr>
<td>0.3</td>
<td>0.180</td>
<td>0.180</td>
<td>0.148(5)</td>
<td>13.05(5)</td>
<td>0.025(5)</td>
</tr>
<tr>
<td>0.4</td>
<td>0.190</td>
<td>0.154(29)</td>
<td>12.98(70)</td>
<td>0.015(8)</td>
<td></td>
</tr>
</tbody>
</table>

\( n \): average number of 3d electrons; IS: isomer shift; \( \mu H_{hf} \): magnetic hyperfine field; QS: quadrupole interaction parameter.

6. Summary

The 3d subbands of the starting compound Dy(Mn\(_{6.4}\)Fe\(_{6-x}\)) of the Dy(Mn\(_{6-x}\),Al\(_x\)Fe\(_{6-y}\)) series are filled-up only partially and both are far away from their completeness. The value of the \(^{57}\)Fe magnetic hyperfine field observed for the Dy(Mn\(_{6-x}\),Al\(_x\)Fe\(_{6-y}\)) belongs to the left branch of the 3d/3d Slater-Pauling curve (Fig. 6, line 1) and lies at a considerable distance from the top area of the \( \mu H_{hf}(n) \) fields (curve 1). The Mn/Al substitution in the series Dy(Mn\(_{6-x}\),Al\(_x\)Fe\(_{6-y}\)) induces strong changes in the 3d band whereas the contribution of iron remains constant across the series.

As well as for the Fe/Al substitution, the Mn/Al substitution is expected to introduce a number of changes in the 3d band [17,18]. At first, there is no doubt that the Mn/Al substitution should change the Fermi energy, the width of bands and the energy shift between subbands [17,18].

The number of manganese atoms in the transition metal sublattice is reduced with \( x \) and simultaneously the MgCu\(_2\)-type crystal lattice parameter \( a \) (Table 1) and thus the distance \( d_{M-M} \) is reduced with 3d electron density at the iron atoms area increase with \( x \) [10,14,29].

It is already known that an increase of the 3d electron density at a given 3d atom (particularly iron atom) leads to a rise of the isomer shift observed at \(^{57}\)Fe [29]. Fig. 7 shows a practically linear correlation between the isomer shift IS(\( n \)) and the crystal volume \( V(3d) \) calculated per atom which supports the above ideas, as discussed elsewhere [12].

The next main problem to discuss below is the \( \mu H_{hf}(n) \) dependence. The reduction of the magnetic hyperfine field against the decreasing \( n \) (Fig. 6, curve 3) can be qualitatively related to the rigid band model [17,18]. Although the formally calculated number of 3d electrons per transition metal sites decreases with the Al content, it seems that in fact there is no a considerable 3d electron density at the Al.
atoms, if any. A similar problem was discussed previously [12]. It seems reasonable to assume that the 3d electrons reside mainly at the transition metal atoms area and that their 3d electron density $\rho_{3d} = \rho_{3d}^+ + \rho_{3d}^-$ per atom is presumably constant across the series. The $\rho_{3d}^+$ and $\rho_{3d}^-$ densities correspond to the spin-up and spin-down subbands, respectively.

The Mn/Al substitution reduces the average number of magnetic nearest neighbors surrounding the probed Fe atom and thus reduces the energy shift $\Delta E \sim \sum (\mu_B M) \delta_{M-M}$ (summation over magnetic nearest neighbors) between the 3d subbands, where $\delta_{M-M}$ is an exchange integral, and presumably also lowers the Fermi level $E_F$. In effect, the 3d electrons should become gradually redistributed over the 3d subbands and the difference between the $\rho_{3d}^+$ and $\rho_{3d}^-$ densities should become reduced step by step with $x$. Consequently, the magnetic moment $\mu_{Mn}$ of the 3d atom and thus the magnetic hyperfine field $H_{hf}$ should also decrease and finally the 3d/3p branch of the Slater–Pauling curve is observed (Fig. 3, curve 3). Comparing the magnetic ordering temperature of DyFe$_2$ ($T_C = 635$ K [1,2]) and the magnetic ordering temperature of Dy(Mn$_{y}$Fe$_{1-y}$)$_2$ ($T_C = 395$ K [30]) it can be concluded that the exchange integral $J_{Fe-Fe}$ has a considerably higher value as compared to the $J_{Fe-Mn}$ exchange integral. Thus the reduction of the energy shift $\Delta E$(Mn/Al) caused by the Mn/Al substitution is lower as compared to the reduction of the energy shift $\Delta E$(Fe/Al) enforced by the Fe/Al substitution.

As a result the $\mu_B H_{hf}(n)$ curve observed for the series Dy(Mn$_{y}$Fe$_{1-y}$)$_2$ (Fig. 3, curve 3) is situated above the $\mu_B H_{hf}(n)$ curve observed for the series Dy(Mn$_{y}$Fe$_{1-y}$)$_2$ (Fig. 3, curve 2).

Since there is no satisfactory background to predict, for example, the change in position of the subbands in relation to the Fermi level $E_F$, and the 3d electron densities $\rho_{3d}^+$, $\rho_{3d}^-$ and $\rho_{3d}$ are unknown yet, at present a more exhaustive discussion is impossible. In fact, the electronic structures of certain rare earth-transition metal compounds were previously studied theoretically and numerically and the band structures were proposed, for instance, in Refs. [31–33]. However, the systematic theoretical and numerical studies of the band structure of the 3d/3d substituted series and especially of the new 3d4s/3p substituted series are unknown yet. Thus for a more precise discussion, a knowledge of the band structure of the Al-substituted intermetallic series is necessary. For this purpose future sound theoretical and numerical studies would be helpful.

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References


Fig. 7. The correlation between the isomer shift IS and the average volume \textit{v} per atom for the series Dy(Mn$_{y}$Fe$_{1-y}$)$_2$: \textit{x}-values belonging to the corresponding experimental points are added.