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MAGNETIC INTERACTION AND CRYSTAL FIELD IN $\text{R}_2\text{Fe}_{14}\text{C}$ AND RELATED COMPOUNDS

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Abstract. - The magnetic interaction constant and the crystal field parameter $B_0^2$ are determined from $^{57}\text{Fe}$, $^{161}\text{Dy}$, $^{166}\text{Er}$ and $^{169}\text{Tm}$ Mössbauer measurements. A comparison has been made with other rare earth iron and cobalt rich intermetallics.

Ternary rare earth compounds of the composition $\text{R}_2\text{Fe}_{14}\text{C}$ have the same tetragonal structure as $\text{R}_2\text{Fe}_{14}\text{B}$. The unit cell contains two different types of R sites and six different types of Fe sites. Therefore this study should be regarded as a continuation of earlier measurements on the $\text{R}_2\text{Fe}_{14}\text{B}$ compounds [1, 2].

$^{57}\text{Fe}$ Mössbauer spectra of $\text{Dy}_2\text{Fe}_{14}\text{C}$, $\text{Er}_2\text{Fe}_{14}\text{C}$ and $\text{Tm}_2\text{Fe}_{14}\text{C}$ show a very close resemblance with the spectra of their $\text{R}_2\text{Fe}_{14}\text{C}$ counterparts as will be published elsewhere [3].

The $^{161}\text{Dy}$ and $^{166}\text{Er}$ spectra of $\text{Dy}_2\text{Fe}_{14}\text{C}$ and $\text{Er}_2\text{Fe}_{14}\text{C}$ measured at $T = 4.2$ K are both slightly asymmetrically broadened and subsequently no clear indication can be found whether the two non-equivalent rare earth sites behave different. A representative spectrum of $\text{Dy}_2\text{Fe}_{14}\text{C}$ is shown in figure 1. However in the case of the $^{169}\text{Tm}$ spectra of $\text{Tm}_2\text{Fe}_{14}\text{C}$ the two non-equivalent sites are recognizable. The hyperfine fields in $\text{Dy}_2\text{Fe}_{14}\text{C}$ and $\text{Er}_2\text{Fe}_{14}\text{C}$ at $T = 4.2$ K are $617 \pm 6$ and $832 \pm 7$ T, respectively. In the case of $\text{Tm}_2\text{Fe}_{14}\text{C}$ the hyperfine fields of the two sites are $750 \pm 3$ and $761 \pm 3$ T. All these values are about 50 T larger than the free ion values. This difference has been ascribed to transferred hyperfine fields and is about the same as in $\text{R}_2\text{Fe}_{14}\text{B}$ [1, 2]. So it can be inferred that the crystal field interaction in these compounds is substantially smaller than the exchange interaction. Therefore we have determined the magnetic coupling constants from the temperature dependence of the $^{161}\text{Dy}$ Mössbauer spectra. Neglecting the weak Dy-Dy interaction with respect to the Dy-Fe interaction one may describe the Dy sublattice magnetization with the Hamiltonian $H = -g_J \mu_B H_m J_z$, where the molecular field $H_m$ can be written as

$$H_m = 2Z_1 J_{RM} \left(1 - b T^2\right) S_M (g_J - 1) / g_J \mu_B.$$  (1)

Here $H_m$ corresponds to a c-axis anisotropy as was observed in $\text{Dy}_2\text{Fe}_{14}\text{C}$. The number of Fe neighbours of the Dy atoms is represented in equation (1) by $Z_1$ and the R-Fe coupling constant is represented by $J_{RM}$. In equation (1) it has furthermore been assumed that the temperature dependence of Fe spins can be given by $S_M (T) = \left(1 - b T^2\right) S_M$, as was found in other R-Fe compounds of similar composition [4]. We have used equation (1) to calculate the temperature dependence of the effective hyperfine field $H_{eff}$ and the quadrupole splitting, $QS = 1/2 e^2 q Q$, by means of

$$H_{eff} (T) = H_{eff} (0) \langle J_s \rangle_{av} / J$$  (2)

$$QS (T) = QS (0) \left\{3 J_z^2 - J (J + 1)\right\}_{av} / J (2 J - 1) + QS_{latt}$$  (3)

where the subscript $av$ means the thermal average and $QS_{latt}$ the lattice contribution. As shown in more detail elsewhere [3], a fit through the experimental data points with the formulas (2) and (3) gives a value of $H_m = 184$ T for $\text{Dy}_2\text{Fe}_{14}\text{C}$. In the crystal structure of $\text{R}_2\text{Fe}_{14}\text{B}$ the R atoms have 18 nearest neighbour Fe atoms on the average. From the $^{57}\text{Fe}$ Mössbauer data it appears that $S_{av} = 1.05$. Then equation (2) leads to a value

$$J_{RM}^{(2)} = (-1.8 \pm 0.1) \times 10^{-22} \text{ J}$$

for the coupling constant between the R and Fe spins, which is the same as found for $\text{Dy}_2\text{Fe}_{14}\text{B}$ [1].

Alternatively one may also obtain an estimate of $J_{RM}$ from a mean field analysis of the bulk magnetic properties of the $\text{R}_2\text{Fe}_{14}\text{C}$ compounds. In the mean-field approximation the Curie temperature can be expressed as

$$3k T_C = a_{MM} + (a_{MR}^2 + 4 a_{RM} a_{MR})^{1/2}$$  (4)

where $a_{MM} = Z J M S_M (S_{M+1})$, and

$$a_{RM} a_{MR} = Z_1 Z_2 S_M (S_{M+1}) (g_J - 1) J (J + 1)^2 J_{RM}^2.$$  (5)

From the crystal structure of $\text{R}_2\text{Fe}_{14}\text{B}$ it follows that

![Fig. 1. $^{161}\text{Dy}$ Mössbauer spectrum of $\text{R}_2\text{Fe}_{14}\text{C}$ measured at $T = 4.2$ K.](image)
Table I. - For the meaning of the different parameters, see text.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Z</th>
<th>Z₁</th>
<th>Z₂</th>
<th>Sₘ</th>
<th>Jₜₜ (10⁻²² J)</th>
<th>J₂₉ (10⁻²² J)</th>
<th>J₃₉ (10⁻²² J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R₂Fe₁₀V₂</td>
<td>8</td>
<td>17</td>
<td>2</td>
<td>0.75</td>
<td>9.5</td>
<td>-2.2</td>
<td>-2.0</td>
</tr>
<tr>
<td>R₂Fe₁₇</td>
<td>10</td>
<td>19</td>
<td>2</td>
<td>1.0</td>
<td>3.2</td>
<td>-1.4</td>
<td>-1.2</td>
</tr>
<tr>
<td>R₂Fe₁₄B</td>
<td>10</td>
<td>18</td>
<td>2.5</td>
<td>1.1</td>
<td>4.8</td>
<td>-1.4</td>
<td>-1.8</td>
</tr>
<tr>
<td>R₂Fe₁₄C</td>
<td>10</td>
<td>18</td>
<td>2.5</td>
<td>1.05</td>
<td>4.8</td>
<td>-1.5</td>
<td>-1.8</td>
</tr>
<tr>
<td>R₂Co₁₇</td>
<td>10</td>
<td>19</td>
<td>2</td>
<td>0.8</td>
<td>21.0</td>
<td>-</td>
<td>-1.4</td>
</tr>
<tr>
<td>RCo₅</td>
<td>8.5</td>
<td>18</td>
<td>3.5</td>
<td>0.75</td>
<td>18.0</td>
<td>-</td>
<td>-2.1</td>
</tr>
</tbody>
</table>

Each R has an average number of Z₁ = 18 Fe nearest neighbour atoms while each Fe atom has an average number of Z₂ = 2.5 R nearest neighbour atoms and an average number of Z = 10 Fe nearest neighbours. From Tc = 495 K (Lu₂Fe₁₄C) substituted in equation (5) one finds Jₜₜ = 4.8 x 10⁻²² J. With this value, Tc = 630 K and J = 7/2 for Gd₂Fe₁₄C, we find by means of equation (5) a value for the R-M coupling constant equal to J₂₉ = -1.5 x 10⁻²² J, which is slightly lower than the value J₀⁻²² = -1.8 x 10⁻²² J derived from the ¹⁶¹ Dy Mössbauer spectra.

In table I we give also the results of other rare earth iron and cobalt rich compounds. The values Sₘ and Tc of the corresponding non magnetic rare earth and Gd compounds are taken from reference [5]. The procedure followed is the same as for the R₂Fe₁₄C compounds. Some of the results have been published earlier [1, 4, 6, 7]. In case of DyCo₅ and Dy₂Co₁₇, Sₘ has been taken constant below 300 K. Since no clear De Gennes behaviour has been found for the Curie temperatures of the RCo₅ or R₂Co₁₇ compounds [5], the J₂₉ values could not be determined by a mean field analysis.

Since for all the compounds under study we have found for the 4f-contribution of the hyperfine fields the free ion value, we expect for the electric quadrupole splitting the same. The measured values of 1/2e²qQ at T = 4.2 K are 5.4 ± 0.5 cm/s and 600 ± 0.5 cm/s for Dy₂Fe₁₄C and Er₂Fe₁₄C respectively. For Tm₂Fe₁₄C the two values of 1/2e²qQ are 15.1 ± 0.3 and 13.5 ± 0.3 cm/s. These results are in reasonable agreement with those of the borides [1, 2, 8]. The deviation from the free ion value of the quadrupole splitting has been attributed to the lattice contribution of which we can determine the crystal field term B₀⁰ as shown earlier [6]. The lattice contribution of the electric quadrupole splitting is Q₀ = -1/2eV² q₀ where Q is the quadrupole moment of the nucleus. From reference [6] it appears, that eV² q₀ ~ B₀⁰. In this way we calculate for compounds with a c-axis anisotropy the crystal field parameters B₀⁰. That is the case for Dy in R₂Fe₁₄B and R₂Fe₁₄C and for Tm in the others. As shown before this is not possible for compounds with a basal plane anisotropy [2], since then the asymmetry is of importance. The results are given in table II.

From table II it is clear that the B₀⁰ term is somewhat low for R₂Fe₁₇ and R₂Fe₁₀V₂ compounds compared to R₂Fe₁₄C. The fairly large B₀⁰ values in the latter compounds combined with the properties given in table I make them possible candidates for permanent magnet purposes. In fact no substantial differences in the physical parameters between R₂Fe₁₄C and R₂Fe₁₄B are found.

Table II. - The determined values of B₀⁰ (K) for rare earth iron and cobalt rich compounds. In the compounds with two different R sites, they are indicated a and b.

<table>
<thead>
<tr>
<th>Compound</th>
<th>B₀⁰(K)</th>
<th>ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TmFe₁₀V₂</td>
<td>&lt;0.3 expected to be negative</td>
<td>6</td>
</tr>
<tr>
<td>Tm₂Fe₁₇</td>
<td>a: -0.5 ± 0.3</td>
<td>b: +0.5 ± 0.3</td>
</tr>
<tr>
<td>Dy₂Fe₁₄B</td>
<td>a&amp;b average: -1.1 ± 0.5</td>
<td>1</td>
</tr>
<tr>
<td>Dy₂Fe₁₄C</td>
<td>a&amp;b average: -1.7 ± 0.5</td>
<td>-</td>
</tr>
<tr>
<td>Tm₂Co₁₇</td>
<td>a: -0.8 ± 0.2</td>
<td>b: -0.3 ± 0.2</td>
</tr>
<tr>
<td>TmCo₆1.1</td>
<td>-1.1 ± 0.2</td>
<td>-</td>
</tr>
</tbody>
</table>