MAGNETIC PROPERTIES OF THE INTERMETALLIC COMPOUNDS RFe2

K. Buschow, R. Van Stapele

To cite this version:

HAL Id: jpa-00214062
https://hal.archives-ouvertes.fr/jpa-00214062

Submitted on 1 Jan 1971

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
MAGNETIC PROPERTIES OF THE INTERMETALLIC COMPOUNDS RFe₂

K. H. J. BUSCHOW and R. P. van STAPELE

Résumé. — Nous avons déterminé les aimantations à saturation à 4.2 K, la température de Curie et les paramètres de la maille pour un certain nombre de composés intermétaux du type RFe₂ (R = Ce, Sm, Gd, Tb, Dy, Ho, Er, Y, Zr). Le comportement magnétique des composés R₂Yₓ₋₁Fe₂ (R = Gd, Tb, Er, Ce) a été étudié en fonction de x. On discute les moments variables du Fe dans les composés RFe₂ et l'absence d'une température de compensation dans la variation thermique de l'aimantation des composés RFe₂ (R = Gd, Tb, Dy, Ho).

Abstract. — For a number of compounds RFe₂ (R = Ce, Sm, Gd, Tb, Dy, Ho, Er, Y, Zr) the lattice constant, the saturation moment at 4.2 K and the Curie temperature have been determined. The magnetic properties of the compounds R₂Yₓ₋₁Fe₂ for R = Gd, Tb, Er and Ce have been studied as a function of composition. The variable iron moment in the compounds RFe₂ is discussed in terms of a non-saturated d-band magnetization. It is shown that the absence of a compensation point in the temperature dependence of the magnetization for R = Gd, Tb, Dy and Ho is a result of a relatively strong negative R-Fe interaction.

1. Introduction. — Investigations of the magnetic properties of several series of rare-earth iron compounds [1-4] have shown that the rare earth spin moment and the iron moment couple antiparallel and that in general the Curie temperatures of these compounds decrease with increasing iron concentration. The present study will be restricted to compounds of the cubic C15 structure so that variations of the magnetic properties arising as a cause of differences in coordination number of the iron atoms can be left out of consideration. The moments of the iron atoms in the C15 compounds seem to be strongly variable and in some cases a strong enhancement of the iron moment occurs due to the polarizing influence of the rare earth spin. Only for some of those rare earth iron compounds, in which the rare earth atoms have their total moment coupled antiparallel to the iron moment, a compensation point in the temperature dependence of the magnetization is observed. This will be explained by taking into account a proper balance between the iron- and rare earth moments and the relative strength of the exchange interaction in these compounds.

2. Experimental. — Apart from the compound SmFe₂ the samples used in this investigation were prepared by arc melting from 99.9 % pure starting materials followed by vacuum annealing. The compound SmFe₂ was prepared by sealing the constituent metals into a Mo container, heating until reaction had occurred and vacuum annealing at 600°C during 4 weeks. The magnetization σ was measured on powdered materials by means of a null coil pendulum magnetometer.

3. Results and discussion. — The experimental data regarding lattice constants, saturation moments per formula unit RFe₂ and the Curie temperatures for a number of binary RFe₂ compounds are summarized in Table I. We have in addition also studied the magnetic properties of four series of ternary compounds: GdₓY₁₋ₓFe₂, TbₓY₁₋ₓFe₂, ErₓY₁₋ₓFe₂ and CeₓY₁₋ₓFe₂. As an example, the temperature dependence of the magnetization is shown for the Er compounds (Fig. 1). It is seen that these curves exhibit compensation points if x > 0.4. In the Gd compounds a compensation point is observed for x = 0.5 : for higher x values (x = 0.75, 0.80, 0.90 and 1.0) compensation points are not observed. Similar, in the Tb compounds a compensation point is present for x = 0.4 but absent in compounds with larger x values : x = 0.70, 0.80, 0.90 and 1.0. More details for the observed σ vs T curves of the Gd- and Tb compounds are given in Ref. [5]. The compounds CeₓY₁₋ₓFe₂ are ferromagnetic and show no compensation points.

The variation of the Curie temperature Tc and saturation moment M with composition is shown for the compounds GdₓY₁₋ₓFe₂ in figure 2. The variation of M with composition reflects the antiparallel coupling of the Fe and Gd moments ; the variation in Tc

Table I

<table>
<thead>
<tr>
<th>Compound</th>
<th>Lattice constant a (Å)</th>
<th>Saturation moment M (μB/mole)</th>
<th>Curie temperature Tc (OK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SmFe₂</td>
<td>7.417</td>
<td>2.75</td>
<td>676</td>
</tr>
<tr>
<td>GdFe₂</td>
<td>7.369</td>
<td>2.80</td>
<td>785</td>
</tr>
<tr>
<td>TbFe₂</td>
<td>7.347</td>
<td>4.72</td>
<td>711</td>
</tr>
<tr>
<td>DyFe₂</td>
<td>7.325</td>
<td>5.50</td>
<td>635</td>
</tr>
<tr>
<td>HoFe₂</td>
<td>7.304</td>
<td>5.50</td>
<td>612</td>
</tr>
<tr>
<td>ErFe₂</td>
<td>7.283</td>
<td>4.80</td>
<td>590</td>
</tr>
<tr>
<td>TmFe₂</td>
<td>7.247 (*)</td>
<td>2.52 (*)</td>
<td>610 (*)</td>
</tr>
<tr>
<td>YFe₂</td>
<td>7.363</td>
<td>2.90</td>
<td>545</td>
</tr>
<tr>
<td>LuFe₂</td>
<td>7.217 (*)</td>
<td>2.97 (*)</td>
<td>610 (*)</td>
</tr>
<tr>
<td>CeFe₂</td>
<td>7.303</td>
<td>2.59</td>
<td>230</td>
</tr>
<tr>
<td>ZrFe₂</td>
<td>7.074</td>
<td>3.10 (*)</td>
<td>625</td>
</tr>
</tbody>
</table>

(*) Ref. [7].
(’) Ref. [8].
(’) Ref. [9].
Magnetic properties of the intermetallic compounds RFe$_2$

Fig. 1. — Temperature dependence of the magnetization for some Er$_x$Y$_{1-x}$Fe$_2$ compounds obtained in a magnetic field of 9 kOe.

Fig. 2. — Curie temperature ($T_c$), saturation moments at 4.2 °K ($M$) and moment per iron atom ($M_{Fe}$) as a function of composition ($x$) for some compounds of the type Gd$_x$Y$_{1-x}$Fe$_2$.

Fig. 3. — Curie temperatures ($T_c$), saturation moments at 4.2 °K ($M$) and moment per iron atom ($M_{Fe}$) as a function of composition ($x$) for some compounds of the type Ce$_x$Y$_{1-x}$Fe$_2$.

reflects the increasing Gd-Fe and Gd-Gd interactions. Also shown in this figure is the variation of the iron moment $M_{Fe}$ with composition, which is seen to be constant over a fairly large region of $x$ values but is strongly enhanced above $x = 0.8$. These iron moments have been obtained from the values given for the saturation moment $M$ after substraction of the free ion value $gS = 7/2$ of the Gd moments. A similar variation with composition of the quantities $T_c$ and $M$ has been observed for the compounds Tb$_x$Y$_{1-x}$Fe$_2$ and Er$_x$Y$_{1-x}$Fe$_2$ (see Ref. 5). The same characteristic constant behaviour of the iron moment from $x = 0$ to about $x = 0.8$ becomes also manifest in these compounds if account is taken of a small reduction of the Tb and Er moments due to the presence of crystal fields. The variation of $T_c$ and $M$ with composition for the compounds Ce$_x$Y$_{1-x}$Fe$_2$ is shown in figure 3. It follows from the lattice constant of CeFe$_2$ with respect to those of the other rare earth iron compounds RFe$_2$ in Table I that Ce in CeFe$_2$ is tetravalent and does not carry a magnetic moment. Replacement of Y by Ce in YFe$_2$ therefore comes essentially to an increase of the conduction electron concentration. It is seen in figure 3 that $T_c$ decreases considerably with $x$ whereas the iron moment remains constant over an appreciable region of $x$ values, but decreases for large $x$.

The experimental results regarding $M_{Fe}$ and $T_c$ can be summarized as follows: 1. $M_{Fe}$ and $T_c$ are enhanced by the rare earth moment. The enhancement of $M_{Fe}$ is far from being proportional to the expectation value of the rare earth's spin moment.

2. $M_{Fe}$ and $T_c$ are enhanced by lattice contraction. This follows from a comparison of the data shown in Table I for YFe$_2$ and LuFe$_2$ and also from a comparison of the data for CeFe$_2$ and ZrFe$_2$ (Ce and Zr are both tetravalent).

3. $M_{Fe}$ and $T_c$ are reduced by an increase in the valence electron concentration. This follows from a comparison of the data given for YFe$_2$ and CeFe$_2$; the lattice contraction in CeFe$_2$ with respect to YFe$_2$ is only moderate and is not able to compensate for the former reduction. The above results are consistent with a model in which the d-band magnetization is unsaturated and in which the Fermi level resides in a region of a low density-of-states [4, 5]. This region can be abandoned by an increase in the exchange energy which governs the splitting between the spin-up and spin-down Fermi levels. This becomes possible either by spin polarization of the Fe moments through the rare earth moments or by lattice contraction which probably results in a larger Fe-Fe interaction.

The absence of compensation points in some of
the compounds $RFe_2$ and $R,Y_{1-x}Fe_2$ can fairly well be understood by a molecular field model with the iron moments coupled antiparallel to the rare earth spin moments. It can be shown that no compensation point will appear in the $\sigma$ vs $T$ curve unless

$$T_\sigma > T_{\text{comp}} = Bg(g - 1)J(J + 1)x + \theta.$$  

For the constant $B$ we derived the value $31.0$ [5]. $\theta$ is the contribution to the asymptotic Curie temperature due to $R-R$ exchange which can be estimated from the magnetic data [6] of the isostructural $RNi_2$ compounds.

Inserting $T_{\text{comp}} \approx T_c$ we estimate $x_m = 0.7$ both in the case of $Gd,Y_{1-x}Fe_2$ and $Tb,Y_{1-x}Fe_2$. In agreement with this value for $x_m$ we do not observe compensation points in the compositions $x = 1.0, 0.9, 0.8$ and $0.75$ for $Gd,Y_{1-x}Fe_2$ and $x = 1.0, 0.9, 0.8$ and $0.70$ for $Tb,Y_{1-x}Fe_2$, while they are present in $Gd_{0.5}Y_{0.5}Fe_2$ and $Tb_{0.4}Y_{0.6}Fe_2$. Using the same arguments in the case of $Dy,Y_{1-x}Fe_2$ and $Ho,Y_{1-x}Fe_2$ we find that the Dy and the Ho concentration should be less than 0.7 and 0.8 respectively in order to give a compensation temperature below $T_c$. This explains the absence of compensation points in $DyFe_2$ and $HoFe_2$, $TmFe_2$ finally is expected to have a compensation point, which agrees with experiment [1].

For samarium one has $J = L - S$ as a ground state which means that in $SmFe_2$ the iron moment and the Sm moment should couple parallel. The expectation value of the Sm spin moment is small and the spin polarization of the Fe moment almost negligible. One expects therefore a value for the Fe moment in $SmFe_2$ at $4.2\,^\circ K$ close to $2.90 + 0.71 = 3.61\, {\mu}_B$. The observed moment falls appreciably below this value. This may be explained as follows: In Sm the separation between the $J = 5/2$ and higher multiplets is relatively small. If the exchange fields operative at the Sm site are sufficiently strong, considerable amounts of the excited multiplets will be mixed into the $J = 5/2$ ground state and produce a change in sign of the expectation value of the spin moment [10]. The total (small) Sm moment will now be coupled antiparallel to the Fe moment which explains the low observed value of the saturation moment.

References