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To cite this version:

R. Coehoorn. ELECTRONIC STRUCTURE AND MAGNETISME IN STABLE AND HYPOTHETICAL Y - Fe COMPOUNDS. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-301-C8-302. <10.1051/jphyscol:19888135>. <jpa-00228280>

HAL Id: jpa-00228280
https://hal.archives-ouvertes.fr/jpa-00228280
Submitted on 1 Jan 1988

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ELECTRONIC STRUCTURE AND MAGNETISME IN STABLE AND HYPOTHETICAL Y – Fe COMPOUNDS

R. Coehoorn
Philips Research Laboratories, P. O. Box 80000, 5600 JA Eindhoven, The Netherlands

Abstract. – Ab-initio self-consistent band structure calculations were performed for the stable compounds Y₂Fe₁₇, Y₆Fe₂₃, YFe₃ and YFe₂, and for the hypothetical compounds YFe₁₂ and YFe₅. The variation of the calculated volumes and magnetic moments with the Y-concentration agrees well with the experimental data. However, the absolute values show small but systematic deviations.

Rare earth-transition metal compounds show a wide variety of interesting magnetic properties and phenomena [1]. Whereas the contribution of the rare earth (R) atoms to the magnetic properties can often be understood from the atomic 4f-level structure of the R³⁺ ions, perturbed only slightly by crystal field and exchange interactions, the contribution of the transition metal atoms is determined by the more delocalized 3d-states. In this paper, calculations of this contribution by means of self-consistent ab initio band structure calculations are presented for all existing, and some hypothetical Y-Fe compounds. Yttrium is chemically very similar to the trivalent rare earth atoms, but it has no localized 4f-moment. The calculations of these ferromagnetic compounds were performed using the Augmented Spherical Wave (ASW) method [2]. Within this method, the potential in spheres centered on the atoms, is taken to be spherical. For all calculations we used a ratio we used a ratio rₓ : rₚₓ = 1.35 for the radii of the spheres around Fe and Y atoms. Exchange and correlation were treated within the local spin density functional (LSDF) approximation [3]. The calculations were scalar relativistic. Spin orbit interaction was neglected.

Calculations were performed for the existing compounds Y₂Fe₁₇, Y₆Fe₂₃, YFe₃ and YFe₂, and for the hypothetical compounds YFe₁₂ and YFe₅. From calculations of the total energy at different volumes the theoretical equilibrium volume and the magnetic moments were calculated. In table I these results are compared with the experimental data. The second column gives the Pearson symbol (crystal symmetry and number of atoms per unit cell). Crystal structure data were taken from [4].

The experimental volumes of the unit cell deviate from those given by Vegard’s law (Tab. I). The deviations reflect the Y-Fe chemical binding. With Y₆Fe₂₃ as a notable exception, the deviation varies regularly with the Y-concentration. The volume of YFe₅ was estimated by an interpolation of the experimental volumes. The calculated volumes are systematically 6-7 %, and for YFe₁₂ about 9 % lower than the experimental values. For bcc-Fe this effect was also found in calculations without the spherical approximation to the potential [5]. It can therefore be concluded that the effect is mainly due to the LSDF approximation.

The last two columns show that the calculated average moment per Fe-atom are systematically lower than the experimental moments. In part this is due to the neglect of the orbital moment in the calculations, which is 0.09 μᵣ, for example, in Fe. However, the difference is also related to the underestimate of the volume, which due to the magneto-volume effect leads to an underestimate of the moments. This is illustrated in figure 1 which gives the calculated moments at the

Table I. – Calculated and experimental properties of Y-Fe Compounds. Vᵥₑ₅ is the volume according to Vegard’s law.

<table>
<thead>
<tr>
<th>Pearson symbol</th>
<th>Vₑₓᵖ/Vᵥₑ₅</th>
<th>Vₑ𝑐𝑎𝑙/Vₑₓᵖ</th>
<th>nₑ𝑐𝑎𝑙 (Vₑ𝑐𝑎𝑙) (μᵣ/Fe)</th>
<th>nₑₓᵖ (μᵣ/Fe)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>cl2</td>
<td>1.0</td>
<td>0.939</td>
<td>2.16</td>
</tr>
<tr>
<td>YFe₁₂</td>
<td>t₁₂₆</td>
<td>0.976</td>
<td>0.911</td>
<td>1.71</td>
</tr>
<tr>
<td>Y₂Fe₁₇</td>
<td>h₁₁₉</td>
<td>0.963</td>
<td>0.933</td>
<td>1.83</td>
</tr>
<tr>
<td>YFe₅</td>
<td>h₆₆</td>
<td>0.940</td>
<td>0.935</td>
<td>1.66</td>
</tr>
<tr>
<td>Y₆Fe₂₃</td>
<td>c₁₁₁₆</td>
<td>0.948</td>
<td>0.935</td>
<td>1.78</td>
</tr>
<tr>
<td>YFe₃</td>
<td>h₁₁₂</td>
<td>0.915</td>
<td>0.935</td>
<td>1.52</td>
</tr>
<tr>
<td>YFe₂</td>
<td>c₁₂₄</td>
<td>0.880</td>
<td>0.935</td>
<td>1.36</td>
</tr>
</tbody>
</table>
calculated and experimental volumes, and the experimental moments. In those cases in which the magneto-volume effect is large, as in YFe$_{12}$ and Y$_2$Fe$_{17}$, the underestimate of the moment is larger than in cases like Fe and YFe$_2$ in which the moments are more stable against compression. The large magneto-volume effects can be explained from the densities of states, which show that all Y-Fe compounds are weak ferromagnets. For strong ferromagnets, like the Co-rich Y-Co alloys, we expect a much smaller magneto-volume effect, and hence a better agreement between the calculated and experimental moments.

The volume and the magnetic moment of Y$_6$Fe$_{23}$ are significantly higher than one would expect from an interpolation in the Y-Fe series. This effect is predicted correctly by the calculations. Calculations of the volume of the non-magnetic compounds do not show such a volume effect for Y$_6$Fe$_{23}$. Therefore we conclude that the effect is of magnetic origin, and not due to a less efficient packing in the Y$_6$Fe$_{23}$ structure. From the trends in the relative positions of the calculated and experimental moments, we estimate that the average moment in YFe$_5$ is $1.8 \pm 0.07 \mu_B$.

R-Fe compounds with the ThMn$_{12}$-structure can be stabilized by minor substitutions with a third element like Ti, V, Cr, Mo, W, Si and Al [6]. These materials show a high 3d and 4f magnetocrystalline anisotropy and a Curie temperature well above room temperature, which makes them promising as starting materials for permanent magnets. By extrapolating data for YF$_{12-x}$V$_x$-compounds ($1.5 \leq x \leq 3.5$) [6, 7] the volume and the saturation magnetization of YFe$_{12}$ can be estimated quite accurately. Figure 1 shows that just as for Y$_2$Fe$_{17}$ the average spin moment, calculated at the experimental volume, is very close to the experimental total moment. However, the moment, calculated at the theoretical volume deviates more strongly from the experimental moment than for the other Y-Fe compounds. This deviation is related to the relatively small ratio of the calculated and experimental volumes: 0.911 vs 0.935 for most of the other compounds. The relatively large errors in the calculated volume and average moment might be due to the use of the overlapping spheres approximation for the potential. In the ThMn$_{12}$-structure the potential around the 8(f) and 8(i) sites is expected to be far from spherical. At the experimental volume a Fe-8(i) atom for example has its first Fe-neighbour at 2.41 Å while the 4 second and 4 third nearest neighbours are found at 2.59 Å and 2.65 Å, respectively, in the other Y-Fe compounds the fraction of Fe-sites for which the surrounding is aspherical to the same extent is much smaller.

At the calculated volume the Y, Fe(f), Fe(i) and Fe(j) moments are $-0.25 \mu_B$, $1.40 \mu_B$, $2.00 \mu_B$ and $1.82 \mu_B$, respectively. In agreement with neutron diffraction results on YFe$_{10}$V$_2$ [8] we thus find that the largest moment is found at the 8(i) site.

Fig. 1. – Calculated and experimental average moments per Fe-atom.