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^{57}Fe MÖSSBAUER STUDY OF $\text{RE}_2\text{Fe}_{14}\text{B}$

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Résumé - Nous avons étudié par effet Mössbauer sur le noyau ^{57}Fe des composés $\text{RE}_2\text{Fe}_{14}\text{B}$ à température ambiante et à 4,2 K (RE = Y, Pr, Gd, Tb, Dy et Er). Les paramètres hyperfins dépendent très fortement de la terre rare. Nos résultats indiquent que les champs hyperfins, notamment sur le site $8j_2$, ont une composante anisotrope importante qui est probablement due à l'anisotropie du couplage hyperfin.

Abstract - We have recorded the ^{57}Fe Mössbauer spectra of $\text{RE}_2\text{Fe}_{14}\text{B}$ compounds at room temperature and at 4.2 K (RE = Y, Pr, Gd, Tb, Dy and Er). The hyperfine parameters have a strong rare-earth dependence. The hyperfine fields are strongly anisotropic. This is particularly true for the $8j_2$ site. This anisotropy probably comes from the hyperfine coupling tensor.

I - Introduction

Since the discovery of the permanent magnet properties of the series $\text{RE}_2\text{Fe}_{14}\text{B}/1$, particularly with RE = Pr or Nd, an intensive effort is made to understand the basic physical mechanisms leading to the high anisotropy. It is generally believed that this anisotropy is mainly due to the crystal field acting on the rare earth ion although recently bulk magnetization measurements on a single crystal of $\text{Y}_2\text{Fe}_{14}\text{B}$ indicate that the anisotropy of the iron slab is not negligible /2/.

In this paper we present some preliminary results obtained by ^{57}Fe Mössbauer spectroscopy on $\text{RE}_2\text{Fe}_{14}\text{B}$ with RE = Y, Pr, Gd, Tb, Dy and Er. These results give some clue of the origin of the iron magnetic anisotropy.

II - Experimental results

In fig. 1 we present our Mössbauer data. On each spectrum a weak line is visible at a velocity of about - 0.5 mm/s, even at 4.2 K. It represents about 3-5 % of the spectrum depending on RE. This line is due to a paramagnetic phase, probably $\text{RE}_{14}\text{Fe}_4\text{B}_4$. Apart from the sample with RE = Er, in each spectrum a line at ≈ 6 mm/s with no symmetric twin indicates a substantial quadrupole splitting. From the crystallography we know that there are six different types of iron sites in the $\text{RE}_2\text{Fe}_{14}\text{B}$ structure /3,4,5/ with relative population 16 : 16 : 8 : 8 : 4, 4. In this preliminary analysis we suppose that to one crystallographic site corresponds only one magnetic site. Therefore we have analyzed our data as an overlay of six sextets plus a doublet due to the paramagnetic phase. In the fit procedure the relative population of the sites is kept fixed. We have noticed that if the populations are varied, a better fit is obtained. This shows that our model has to be improved to take into account the possibility that to one crystallographic site may correspond more than one magnetic site. For all the components the quadrupole interaction has been treated in perturbation. We have checked by numerical comparison between spectra computed using the full hamiltonian and the hamiltonian where the quadrupole interaction is taken as a perturbation that the approximation is fully justified.

Because of the complex spectra resulting from the seven sites, the analysis seems to be unambiguous only for three sites for all the samples except for RE = Er where no line exists at velocity ≈ 6 mm/s. The three sites are the two sites with relative population 16 and the site which

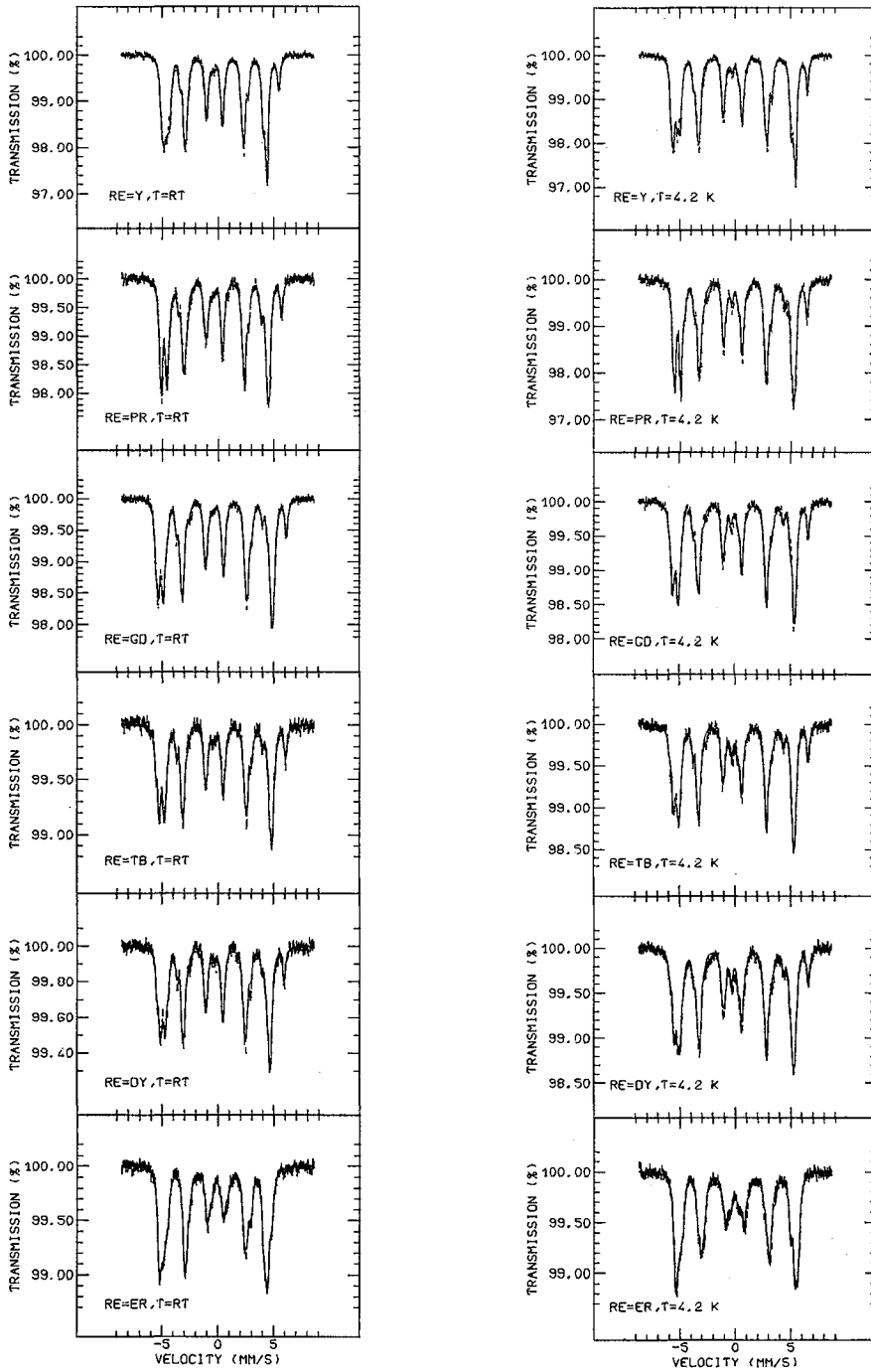


Fig. 1 - ^{57}Fe Mössbauer spectra for $\text{RE}_2\text{Fe}_{14}\text{B}$ at room temperature (RT) and at 4.2 K.

has a relative population 8 and a line at velocity ≈ 6 mm/s. In table 1 we present the parameters extracted from the data. We have distinguished the 16 k_1 and 16 k_2 sites as follows : the 16 k_1 site has a boron as a nearest neighbour whereas it is not the case for the 16 k_2 site. Therefore by charge transfer from the boron to the iron d-band, the iron hyperfine field at the 16 k_1 site should be smaller than at the 16 k_2 site. For the attribution of the asymmetric line to the $8j_1$ site we use an analogy with the RE_2Fe_{17} compounds /6/. For RE = Er we present two set of data for the $8j_1$ site which correspond to the two sites with relative population 8 in the fit procedure. The same arguments have been used by Onodera et al /8/. In addition, studying $Dy_2Fe_{14}B$ hydrides /6/ we give new results which able us to confirm the iron sites assignment. The numbering of the sites corresponds to /5/.

Table 1 - ^{57}Fe hyperfine parameters extracted from the fits shown in Fig. 1. For each rare earth the first (second) line corresponds to room temperature (4.2 K) data respectively. H_{hf} is the hyperfine field, QS the quadrupole splitting and IS the isomer shift relative to a source of ^{57}Co in a Rh matrix at room temperature. \bar{H}_{hf} is the mean hyperfine field over the six iron types of sites. The experimental uncertainties are : $H_{hf} = \pm 3$ kOe, $QS = \pm 0.03$ mm/s and $IS = \pm 0.03$ mm/s.

SITE	16 k_1			16 k_2			8j ₁			\bar{H}_{hf} (kOe)
	H_{hf} (kOe)	QS (mm/s)	IS (mm/s)	H_{hf} (kOe)	QS (mm/s)	IS (mm/s)	H_{hf} (kOe)	QS (mm/s)	IS (mm/s)	
Pr	286	0.33	-0.11	294	0.08	-0.32	336	0.68	-0.02	292
	321	0.47	0.03	333	0.06	-0.17	368	0.77	0.17	328
Gd	302	0.32	-0.15	322	0.15	-0.22	362	0.61	-0.01	312
	326	0.38	0.04	340	0.08	-0.18	375	0.85	0.19	335
Tb	292	0.26	-0.18	314	0.15	-0.26	360	0.59	-0.03	310
	324	0.34	0.05	337	0.10	-0.18	372	0.91	0.19	333
Dy	292	0.25	-0.14	310	0.12	-0.24	353	0.60	-0.05	302
	320	0.32	0.08	333	0.10	-0.19	368	0.95	0.21	329
Er	280	-0.08	-0.33	298	-0.16	-0.28	296	-0.15	0.18	291
							305	-0.43	-0.15	
	310	0.04	-0.02	332	-0.01	0.00	346	0.20	-0.04	327
							340	-0.17	0.33	
Y	261	0.21	-0.19	286	0.17	-0.23	327	0.51	-0.04	284
	311	0.27	-0.06	341	0.18	-0.13	380	0.61	0.10	336

III - Discussion

First we do not consider the Er compound data. The quadrupole splitting (QS) of site $8j_1$ is strong for a metallic compound. In addition the H_{hf} seems to follow a de Gennes law :

$$H_{hf} = \alpha + \beta(g_J - 1)J$$

where α and β are constants and g_J is the Landé factor of the RE. The hyperfine field in the Er compound does not follow this law, particularly at room temperature. It is known that at room temperature the bulk magnetization of the compounds we have studied is parallel to the c-axis except for RE = Er /7/. These results show that the measured hyperfine field is not isotropic. This may have two origins : the dipolar field at the iron site and the anisotropy of the hyperfine coupling tensor. The anisotropy of the $8j_1$ hyperfine field is probably too strong to be due only to the dipolar field. Therefore part of the measured anisotropy comes from the hyperfine coupling tensor. This anisotropy has probably the same origin as the one measured by bulk magnetization on $Y_2Fe_{14}B$. The temperature and the RE dependence of QS may give some information on the local magnetization at the iron sites. For instance, the change of sign of QS for site $8j_1$ for the Er compound compared to the other compounds at room temperature is consistent with the fact that the magnetization is in the basal plane for the Er compound and along the c-axis for the other compounds.

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