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⁵⁷Fe Mössbauer studies of YFe₁₁Ti ($T = 77\text{--}550\text{ K}$)

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Abstract. ⁵⁷Fe Mössbauer effects of YFe₁₁Ti with the ThMn₁₂ structure have been studied in a temperature range of 77–550 K. This material may be considered as the prototype of similar systems with yttrium replaced by a magnetic rare earth. The results show that the largest hyperfine field is on the 8i site and the smallest on the 8f site. The hyperfine fields are 23.5 T, 21.8 T and 20.2 T, the quadrupole splittings are 0.32, –0.17 and 0.27 mm s^{–1} and the spectrum shifts are 0.01, –0.40 and –0.11 mm s^{–1} for the 8i, 8j and 8f sites at room temperature. The quadrupole splittings are 0.29, 0.51 and 0.63 mm s^{–1} and the spectrum shifts are –0.27, –0.48 and –0.31 mm s^{–1} from the paramagnetic spectrum at a temperature of 550 K. Almost all Ti atoms occupy the 8i site according to the subspectral area ratios of 2.9:4.2:3.9 for the 8i, 8j and 8f sites. With increasing temperatures, $H_{\text{HF}}(T)/H_{\text{HF}}(77\text{ K})$ decreases the most slowly for the 8j site and the most rapidly for the 8f site.

1. Introduction

The rare-earth and iron intermetallic compounds with the ThMn₁₂ structure have attracted great interest for possible applications as permanent magnets. The compounds have compositions of RFe_{12–x}M_x, where R represents Y or almost the whole lanthanide series from Nd to Lu, M denotes elements V, Ti, Mo, Cr, W and Si, and x is in the region 1–3.5 [1–3]. The magnetic ordering temperatures of RFe_{12–x}M_x are fairly high. For example, the Curie temperatures are 584 K and 524 K for SmFe₁₁Ti and YFe₁₁Ti respectively [1, 2]. For a given series of RFe₁₁M, the magnetic ordering temperatures vary with the R component approximately according to the de Gennes factor $G = (g - 1)^2 J(J + 1)$. It has been observed that the lowest ordering temperature is for R = Lu and that the highest is for R = Gd [3]. RFe₁₁M with a light rare earth has a fairly high saturation magnetisation, 19.0 $\mu_{\text{B}}\text{FU}^{-1}$ for YFe₁₁Ti and 19.1 $\mu_{\text{B}}\text{FU}^{-1}$ for SmFe₁₁Ti at $T = 1.5\text{ K}$ [4]. The magnetic structures at various temperatures for the RFe₁₁Ti and RFe₁₀V₂ series have been reported by Hu *et al* [5] and Buschow [6]. In a RFe₁₁Ti series all compounds except R = Tb show a uniaxial anisotropy at room temperature. At low temperature the compounds with R = Y, Sm, Gd, Ho, Tm and Lu also have a uniaxial anisotropy; the other compounds have a complex spin structure.

A few papers on Mössbauer spectra of RFe_{12–x}M_x with the ThMn₁₂ structure have been published up to now [7–9]. Wang *et al* [8] reported the Mössbauer spectrum of GdFe₁₀Al₂ at room temperature and indicated that Al occupied the 8f and 8j sites.

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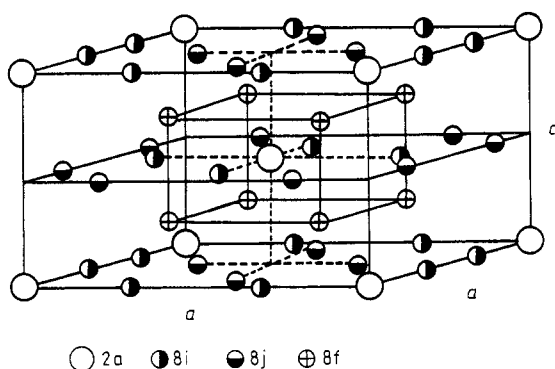


Figure 1. Schematic representation of the ThMn_{12} -type unit cell.

Coey's group studied the spin reorientation of $\text{DyFe}_{11}\text{Ti}$ in a temperature range of 77–300 K with the Mössbauer effect [9].

In order to gain a better understanding of the magnetic properties of YFe_{11}Ti , we measured the Mössbauer spectra in the temperature range of 77–550 K. The assignment of the 8i, 8j and 8f sites, the occupancy of the Ti atoms and the temperature dependence of hyperfine parameters have been investigated.

2. Experiment

A sample of YFe_{11}Ti was prepared by the arc melting of 99.5% pure primary materials under an Ar atmosphere. The sample was identified as a single phase by x-ray diffraction, optical microscope observation and thermomagnetic analysis. It has the tetragonal ThMn_{12} structure with lattice constants of $a = 8.597 \text{ \AA}$ and $c = 4.764 \text{ \AA}$ as determined by diffraction with $\text{Cu K}\alpha$ radiation.

By using the Mössbauer thermal scan method and thermomagnetic analysis the Curie temperature of YFe_{11}Ti was measured to be 525 K. ^{57}Fe Mössbauer spectra of YFe_{11}Ti were taken at temperatures of 77–550 K, with a conventional constant acceleration spectrometer. The γ -ray source was ^{57}Co in a Rh matrix. The calibration was made by using the spectrum of α -Fe at room temperature.

Mössbauer spectra were analysed assuming Lorentzian line shapes. Some constraints were used in the fitting procedure. The positions of the six lines for each subspectrum were determined by the hyperfine field H_{HF} , the quadrupole splitting ε and the spectrum shift δ . The area ratios of the six absorption lines in each sub-spectrum were assumed to be 3 : 2 : 1 : 1 : 2 : 3 because the absorber was a powder with randomly oriented particles and the data analysis indicated that the quadrupole splitting was small. In addition, a doublet was necessary to get a good fit at $T = 470 \text{ K}$, which might be attributed to magnetic relaxation as the sample was close to the Curie temperature.

3. Results and discussions

YFe_{11}Ti has the tetragonal structure with the space group $\text{I}4/\text{mmm}$. Figure 1 illustrates the tetragonal unit cell which contains two formula units, i.e. two R atoms and twenty-

Table 1. The interatomic distances (in Å) and the numbers of adjacent atoms for each site by Yang [10].

Site	8i		8j		8f	2a
8i	2.390 × 1	2.920 × 4	2.664 × 2	2.661 × 2	2.636 × 4	3.104 × 1
8j	2.664 × 2	2.661 × 2	2.711 × 4		2.468 × 4	3.058 × 2
8f	2.636 × 4		2.468 × 4		2.382 × 2	3.265 × 2

four 3d atoms. The R atoms are located on the 2a site and the 3d atoms on the 8i, 8j and 8f sites. The occupancy of each 3d site is eight. The interatomic distance and the number of adjacent atoms for each site are listed in table 1.

Three, four, six and ten subspectra have been tried to fit the Mössbauer spectrum of YFe₁₁Ti. At least four subspectra are needed in order to obtain a good fit. Some typical Mössbauer spectra and their fitted curves using four subspectra are shown in figure 2. The line-widths of the 1st and 6th, the 2nd and 5th and the 3rd and 4th peaks of each sub-spectrum are about 0.6, 0.5 and 0.3 mm s⁻¹ respectively. The broadening of the lines can be attributed to the distribution of adjacent Ti atoms on each site. The hyperfine parameters at *T* = 300 K and 500 K are listed in table 2.

The relative area of the subspectra 1 plus 2 is 26.8%, which is close to 2.9/11. The relative areas of the subspectra 3 and 4 are 37.6% and 35.6%, which are close to 4.2/11 and 3.9/11 respectively. Neutron diffraction has shown that the Ti atoms occupy the 8i site and the occupation numbers of Fe atoms are about 3:4:4 for the 8i, 8j and 8f sites [10]. Hence the subspectra 1 and 2 can be reasonably assigned to the 8i site. The origin of these two subspectra would seem to be the different neighbour configurations of Fe and Ti atoms over the 8i sites. In addition, the 8i site has the most adjacent Fe atoms (11.75 on average), whereas each 8j and 8f site has only nine adjacent Fe atoms. Thus, the largest hyperfine field should be for the 8i site. However, it is difficult to assign properly the subspectra 3 and 4 to the 8j and 8f sites because the numbers of the site occupancies and of the adjacent Fe atoms are the same for the two sites. According to the results of neutron diffraction the magnetic moment of the 8j site is larger than that of the 8f site [10]; hence it is reasonable to assign subspectrum 3 to the 8j site and subspectrum 4 to the 8f site. As a result, the order of the magnitude of the hyperfine fields is: $H_{\text{HF}}(8i) > H_{\text{HF}}(8j) > H_{\text{HF}}(8f)$.

The dependences of the hyperfine parameters on temperature are shown in figures 3 and 4. The values for the 8i site are the average of subspectra 1 and 2. The spectrum shifts for each site decrease with increasing temperature, which is consistent with the second-order Doppler shift. The quadrupole splittings have a linear relationship with temperature below the Curie temperature except those on the 8f site at the temperatures of 77 K and 110 K. We note that the quadrupole splittings below the Curie temperature differ notably from that at 550 K for the 8j and 8f sites, which may be related to the distribution of the polar angles between the principal axis of the electric field gradient tensors and the direction of the hyperfine field below the Curie temperature [11]. Figure 4 shows the dependence of the reduced hyperfine fields $H_{\text{HF}}(T)/H_{\text{HF}}(77\text{ K})$ on the reduced temperatures T/T_f , where $T_f = 525\text{ K}$. With increasing temperature, $H_{\text{HF}}(T)/H_{\text{HF}}(77\text{ K})$ decreases most slowly for the 8j site and most rapidly for the 8f site. It is known that the average distances of the Fe–Fe nearest neighbours are 2.71 Å, 2.60 Å and 2.51 Å for the 8i, 8j and 8f sites respectively in YFe₁₁Ti. The interatomic distances

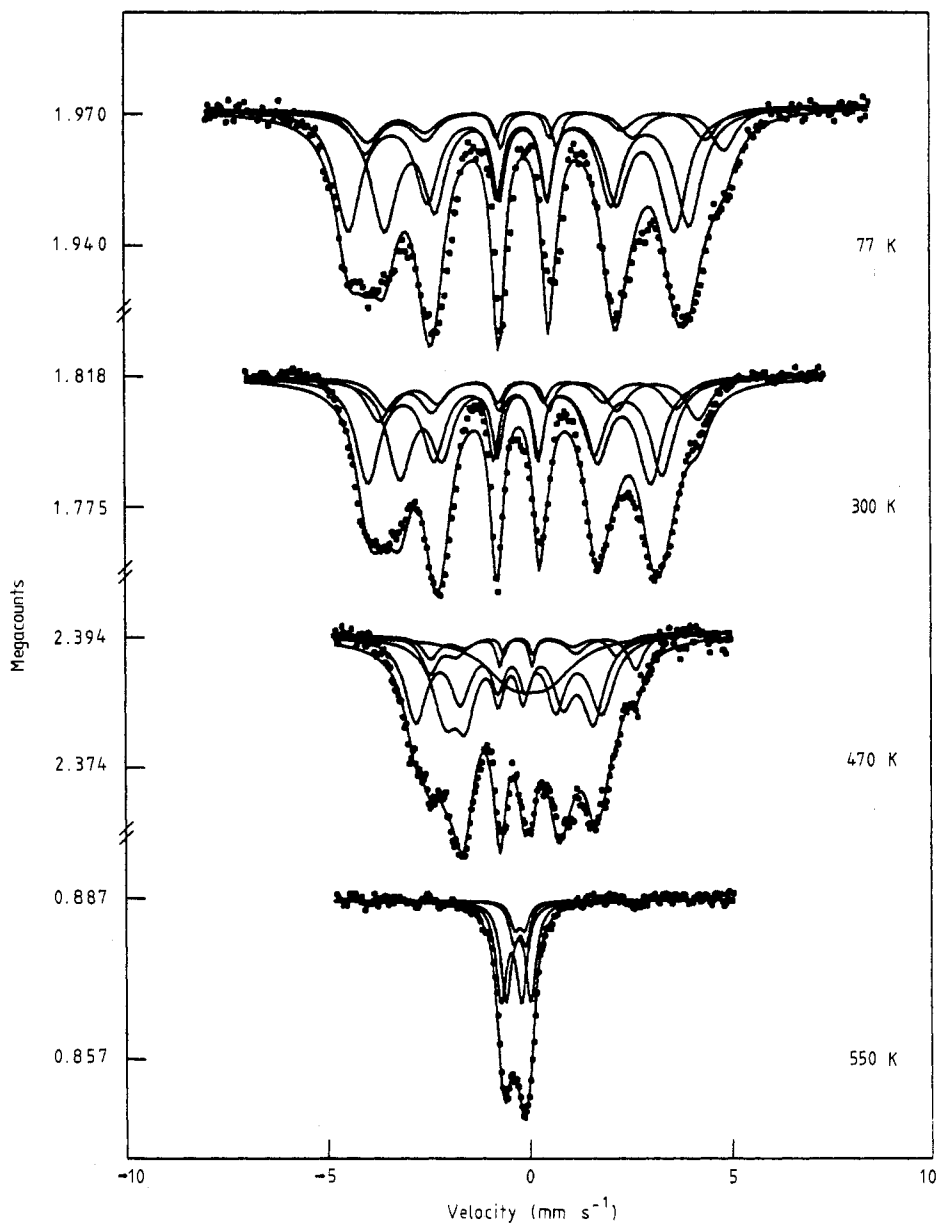


Figure 2. Mössbauer spectra of YFe_{11}Ti and the computer-fitted curves. The sharpness of some lines near their minima is merely an artifact of the computer plotting program used.

between the adjacent atoms cover a large range from 2.382 Å to 2.920 Å (table 1). If the distance is larger than 2.45 Å, the exchange interactions between the adjacent Fe atoms are positive; otherwise, the interactions are negative [12]. The total exchange interaction can be decreased owing to the negative interaction. For the 8f site, the average distance

Table 2. Hyperfine parameters of YFe₁₁Ti. Hyperfine field, H_{HF} ; quadrupole splitting, ϵ ; spectrum shift, δ (relative to the α -Fe at room temperature), and relative area, S . (a) $T = 300$ K. (b) $T = 550$ K.

(a) No	H_{HF} (T)	ϵ (mm s ⁻¹)	δ (mm s ⁻¹)	S (%)
1	24.6	0.35	0.06	15.3
2	22.1	0.27	-0.07	11.5
3	21.8	-0.17	-0.40	37.6
4	20.2	0.27	-0.11	35.6

(b) No	ϵ (mm s ⁻¹)	δ (mm s ⁻¹)	S (%)
1	0.31	-0.27	16.4
2	0.26	-0.27	10.9
3	0.51	-0.48	36.3
4	0.63	-0.31	36.4

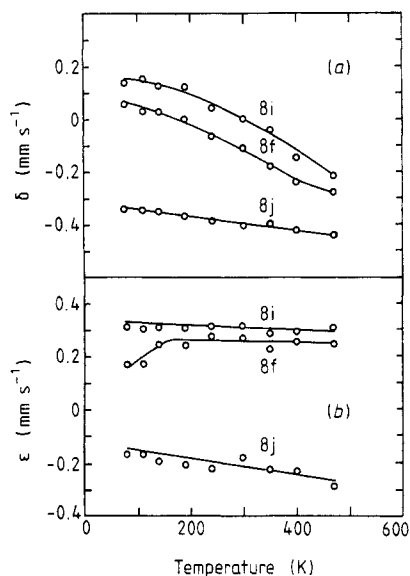


Figure 3. (a) Temperature dependence of the spectrum shifts δ and (b) the quadrupole splitting ϵ in YFe₁₁Ti.

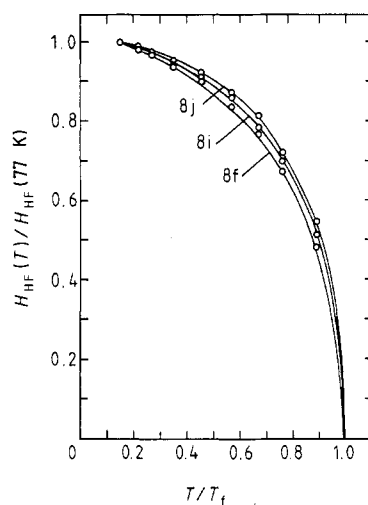


Figure 4. The relationship between the $H_{\text{HF}}(T)/H_{\text{HF}}(77 \text{ K})$ and the T/T_f in YFe₁₁Ti. $T_f = 525$ K; $H_{\text{HF}}(77 \text{ K}) = 26.9$ T, 25.1 T and 23.1 T for the 8i, 8j and 8f sites.

to its adjacent Fe atoms is shortest and two pairs of 8f–8f atoms (distance of 2.382 Å) have negative interactions. We believe that the interaction of the 8f site with its adjacent Fe atoms is weakest. Hence, $H_{\text{HF}}(T)/H_{\text{HF}}(77 \text{ K})$ decreases most rapidly with increasing temperature. The 8i site has the most neighbouring Fe atoms with the largest average distance to its adjacent atoms. The site should have the strongest exchange interaction. However, $H_{\text{HF}}(T)/H_{\text{HF}}(77 \text{ K})$ of the 8i site falls below that of the 8j site. It is known that there is one pair of atoms having a negative interaction (distance of 2.390 Å) for the 8i

site and there is none for the 8j site. Perhaps this causes the interaction at the 8i site to be weaker than that at the 8j site.

4. Conclusion

The hyperfine parameters have been obtained from fits to the Mössbauer spectra for YFe_{11}Ti . The order of the magnitude of the hyperfine fields is: $H_{\text{HD}}(8\text{i}) > H_{\text{HF}}(8\text{j}) > H_{\text{HF}}(8\text{f})$. With increasing temperature, $H_{\text{HF}}(T)/H_{\text{HF}}(77\text{ K})$ decreases most slowly for the 8j site and most rapidly for the 8f site. Ti atoms occupy the 8i site. The quadrupole splittings and the spectrum shifts are almost linear with temperature except for the quadrupole splittings on the 8f site in the temperature range 77–110 K. These results should be useful in the analysis of Mössbauer spectra of similar compounds containing magnetic rare earth atoms.

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