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Dwayne E. Tharp

Gary J. Long

Missouri University of Science and Technology, glong@mst.edu

Oran Allan Pringle

Missouri University of Science and Technology, pringle@mst.edu

Gaya Kanishka Marasinghe

et. al. For a complete list of authors, see https://scholarsmine.mst.edu/chem_facwork/826

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A Mössbauer effect study of $Y_2Fe_{14}B$ and its aluminum solid solutions

Dwayne E. Tharp, Gary J. Long, O. A. Pringle, G. K. Marasinghe, and W. J. James
*Departments of Chemistry and Physics and the Graduate Center for Materials Research,
University of Missouri-Rolla, Rolla, Missouri 65401*

F. Grandjean

Institut de Physique, Universite de Liege, B-4000 Sart Tilman, Belgium

The Mössbauer spectra of $Y_2Fe_{14}B$ have been measured from 85 to 296 K. Analysis of the spectra indicates that the near-neighbor rare-earth atoms directly influence the orientation of the principal axis of the electric field gradient. The hyperfine parameters are very similar to those of $Nd_2Fe_{14}B$, but the internal fields are somewhat smaller at room temperature in the yttrium compound. The Mössbauer spectra of $Y_2(Fe_{1-x}Al_x)_{14}B$, where x equals 0.00, 0.02, 0.04, 0.06, and 0.08, have been measured at 85 K. The average internal hyperfine field in these compounds decreases linearly with increasing aluminum content.

INTRODUCTION

In a detailed analysis of the Mössbauer effect hyperfine parameters for $Nd_2Fe_{14}B$ above its spin reorientation temperature, Grandjean *et al.* found that the positions of the near-neighbor neodymium atoms determine the orientation of the principal axis of the electric field gradient tensor relative to the easy axis of magnetization.¹ In this paper we report a similar analysis for $Y_2Fe_{14}B$ as a function of temperature, demonstrating the general validity of this approach to the analysis of the Mössbauer spectra.

Magnetic measurements² on $Y_2(Fe_{1-x}Al_x)_{14}B$ have shown an increase in the coercivity and anisotropy accompanied by a reduction in the Curie temperature. Aluminum prefers to occupy the $8j_2$ site,^{2,3} apparently because the $8j_2$ site has the largest internal void size of the iron sites. Mössbauer spectra of $Y_2(Fe_{1-x}Al_x)_{14}B$ with x equal to 0.00, 0.02, 0.04, 0.06, and 0.08, have been obtained at 85 K in order to determine the effect of nonmagnetic aluminum in these substituted alloys. The present work thus complements our previous room-temperature work.³

EXPERIMENT

Samples were prepared by arc melting 99.9% pure starting materials, followed by vacuum annealing at 973 K for 6 h. X-ray diffraction patterns indicated single phase materials. Powders used for Mössbauer analysis were prepared by crushing ingots to 400 mesh (0.038 mm^2) under a dry nitrogen atmosphere. Mössbauer effect absorbers were approximately 36 mg/cm^2 thick. Mössbauer spectra were obtained at ambient temperature and 85 K by using a Harwell constant acceleration spectrometer, a room-temperature rhodium matrix cobalt-57 source, and room-temperature α -iron foil for calibration.

MÖSSBAUER SPECTRAL ANALYSIS

In the analysis of the $Y_2Fe_{14}B$ Mössbauer spectra as a function of temperature, the approximate positions of the six lines of each sextet were used as a starting point to determine the internal hyperfine field, isomer shift, quadrupole interaction, Euler angles, and asymmetry parameter, η , for each

site.⁴ This approach indicates, as expected, that η is small for all but the $16k_2$ site. Thus, each sextet is defined by its relative area, linewidth, isomer shift, hyperfine field, quadrupole interaction, and θ , the angle between the principal axis of the electric field gradient tensor and the easy axis of magnetization. Grandjean *et al.*¹ have shown that appropriate θ values are 6.3° , 45.5° , 2.5° , 11.4° , 0° , and 90° , for the $16k_1$, $16k_2$, $8j_1$, $8j_2$, $4e$, and $4c$ sites, respectively. These angles are determined by the position of the near-neighbor rare-earth atoms and the direction of the magnetic easy axis. Fits using these fixed θ angles are shown in Fig. 1. In these final fits at most 20 parameters are adjusted, namely the total area, one linewidth for all 36 lines, and the isomer shifts, internal fields, and quadrupole interactions for each magnetic sextet.¹ The resulting hyperfine parameters are given in Table I.

Magic angle experiments⁵ indicated the presence of a small amount of texture in our $Y_2Fe_{14}B$ sample, as reflected in area ratios of 3:2.1:1.2:1.3 within each sextet. This texture has not been included in the fits shown in Fig. 1, in which the areas of each sextet are constrained to the theoretical values defined by the Hamiltonian eigenvectors. Our failure to adequately account for the added intensity in the 2, 5 lines results in an overestimate of the area of the 1, 6 lines.

The Mössbauer spectra for the $Y_2(Fe_{1-x}Al_x)_{14}B$ compounds were fit with six magnetic sextets having variable internal hyperfine fields, isomer shifts, quadrupole shifts, linewidths, incremental linewidths, one total absorption area, and one texture parameter, for a total of 32 adjustable parameters. With aluminum substitution, the equivalence of the 36 linewidths has been removed because the transition metal sites may now have different first coordination environments, and thus a distribution of hyperfine parameters for each sextet. Relative areas for all of the magnetic sextets were constrained in the ratio $3:x:1:1:x:3$, where x ranges from 2.0 to 2.2, as a result of some texture in the absorber. The relative sextet areas were constrained in the ratios determined from crystallographic requirements, except that the area for the $8j_2$ site reflects the total aluminum occupation.³ When required, a paramagnetic doublet was incorporated in the fit to account for either traces of an impurity or a superparamagnetic component.

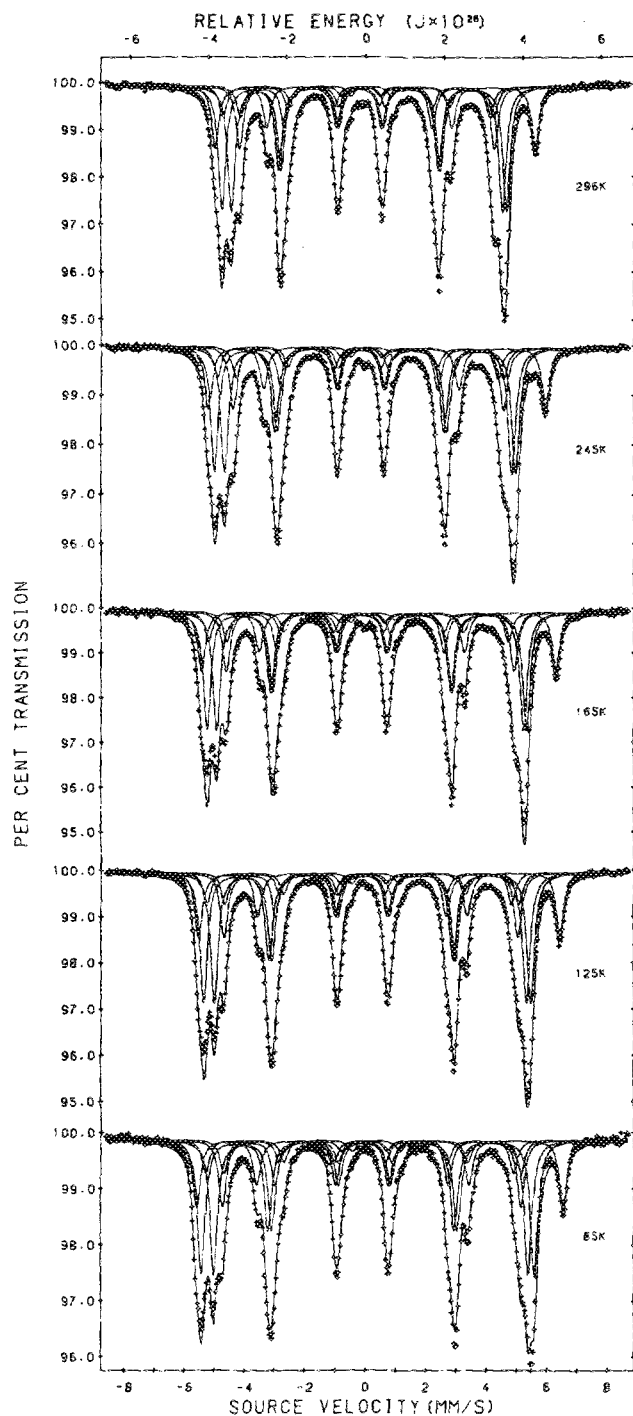


FIG. 1. Mössbauer spectra of $Y_2Fe_{14}B$ as a function of temperature.

RESULTS AND DISCUSSION

The Mössbauer spectra and fits of $Y_2Fe_{14}B$ as a function of temperature are shown in Fig. 1 and the associated hyperfine parameters are given in Table I. The hyperfine fields for each sextet increase smoothly toward their saturation value with decreasing temperature. For each spectral component, the isomer shift also increases with decreasing temperature, consistent with a second order Doppler shift. The quadru-

TABLE I. Temperature dependence of the $Y_2Fe_{14}B$ hyperfine parameters.

Site	T	$16k_1$	$16k_2$	$8j_1$	$8j_2$	$4e$	$4c$
	(K)						
H_{int} (kOe)	296	277	289	261	327	275	255
	285	282	293	265	334	279	257
	245	294	306	277	346	292	268
	205	303	317	287	355	302	277
	165	313	325	295	363	312	288
	125	317	332	301	370	315	293
	85	322	336	306	375	320	296
Isomer shift (mm/s)	296	-0.065	-0.116	-0.089	0.064	-0.025	-0.086
	285	-0.055	-0.103	-0.079	0.097	-0.004	-0.070
	245	-0.025	-0.078	-0.043	0.126	0.030	-0.036
	205	0.003	-0.054	-0.014	0.140	0.062	-0.020
	165	0.026	-0.036	0.010	0.170	0.104	-0.006
	125	0.047	-0.015	0.035	0.196	0.120	0.010
	85	0.068	0.000	0.050	0.217	0.150	0.035
$\frac{1}{2}e^2qQ$ (mm/s)	296	0.232	0.650	0.287	0.546	-0.417	-0.325
	285	0.233	0.692	0.281	0.502	-0.398	-0.350
	245	0.247	0.650	0.289	0.542	0.391	-0.386
	205	0.255	0.676	0.307	0.550	-0.418	-0.364
	165	0.265	0.700	0.310	0.584	-0.443	-0.350
	125	0.260	0.740	0.330	0.584	-0.444	-0.350
	85	0.269	0.748	0.324	0.590	-0.425	-0.350

pole interaction remains virtually constant with temperature for the $16k_1$, $8j_1$, $8j_2$, $4e$, and $4c$ sites, because there is no spin reorientation in $Y_2Fe_{14}B$. The variation in the quadrupole interaction for the $16k_2$ site is not significant because θ is close to the magic angle of 54° . At this angle the quadrupole interaction has no effect on the line positions. Similar trends were observed for all the $Nd_2Fe_{14}B$ hyperfine parameters,¹ with $Nd_2Fe_{14}B$ showing slightly larger hyperfine fields for all sites. The area weighted average hyperfine fields for $Y_2Fe_{14}B$ are 284 kOe at 296 K and 319 kOe at 165 K. In comparison, the values for $Nd_2Fe_{14}B$ are 295 kOe at 296 K and 323 kOe at 155 K. The substitution of yttrium for neodymium reduces the magnetization in $Y_2Fe_{14}B$ as compared to that in $Nd_2Fe_{14}B$, but apparently has little effect on the iron sublattice moments at saturation.

Mössbauer spectra and fits for $Y_2(Fe_{1-x}Al_x)_{14}B$, obtained at 85 K are shown in Fig. 2. The collapse of the magnetization of iron with increasing aluminum substitution is much larger than expected from simple dilution with non-magnetic aluminum.³ Our results at 85 K yield the hyperfine fields, as a function of composition, shown in Fig. 3. The ordering of the different sites is consistent with our previous fits for the room-temperature spectra,³ as well as with our fits for the related $Nd_2(Fe_{1-x}Co_x)_{14}B$ and $Y_2(Fe_{1-x}Co_x)_{14}B$ compounds.⁶ The hyperfine fields for the four largest area sites, the $16k_1$, $16k_2$, $8j_1$, and $8j_2$ sites, are generally consistent with most previous solid solution Mössbauer effect work and also with neutron diffraction studies on the pure iron compounds.⁷ The $8j_2$ site has a large enough void size to accommodate the larger aluminum atom and therefore receives essentially all the available aluminum. Every site except the $8j_2$ and $4c$ sites has at least one $8j_2$ nearest-

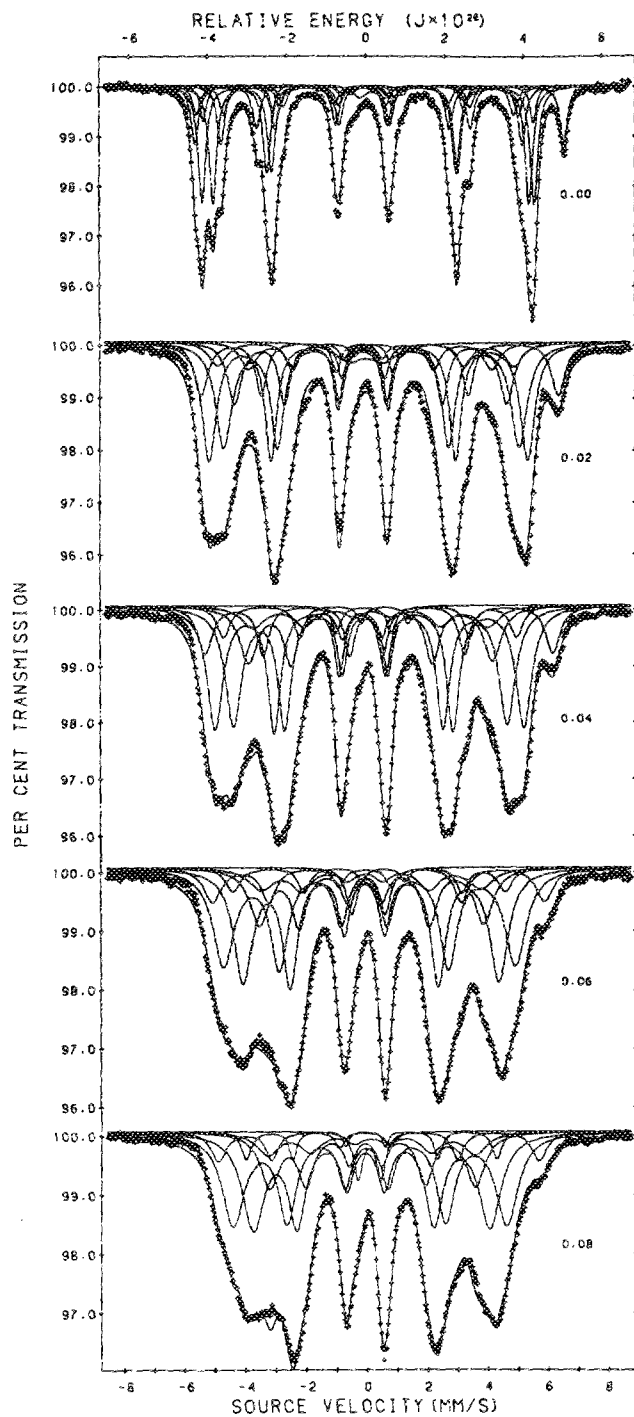


FIG. 2. Mössbauer spectra of $Y_2(Fe_{1-x}Al_x)_{14}B$ obtained at 85 K.

neighbor atom. Because aluminum preferentially occupies the $8j_2$ site, every site except the $4c$ and $8j_2$ sites potentially has an aluminum atom as a near neighbor, and therefore will experience similar environmental changes with aluminum

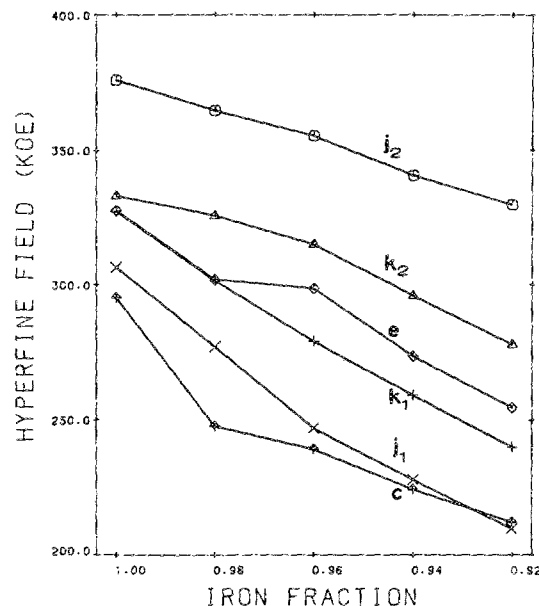


FIG. 3. Variation of the hyperfine fields with composition of $Y_2(Fe_{1-x}Al_x)_{14}B$ at 85 K.

substitution. As a result, the $16k_1$, $16k_2$, $8j_1$, and $4e$ sites have similar linewidths at each composition. As seen in Fig. 3, the $8j_2$ and $4c$ sites exhibit smaller changes in hyperfine field with increasing aluminum content, consistent with room-temperature results.³ The area weighted averages of the hyperfine fields at 296 and 85 K decrease linearly with increasing aluminum content. The slopes and intercepts obtained from linear least-squares fits were found to be -9.0 kOe/% aluminum and 283.2 kOe at 296 K, and -9.6 kOe/% aluminum and 329.6 kOe at 85 K.

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