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Ying-chang Yang

Gary J. Long

Missouri University of Science and Technology, [glong@mst.edu](mailto:glong@mst.edu)

William Joseph James

Missouri University of Science and Technology

R. Yeh

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# Structural and magnetic properties of $Y(Al_{1-x}Fe_x)_{12}$ <sup>a</sup>

Y. C. Yang, G. J. Long, and W. J. James

Graduate Center for Materials Research and Department of Chemistry, University of Missouri-Rolla, Rolla, Missouri 65401

R. Yeh

Department of Physics, The Ohio State University, Columbus, Ohio 43210

In order to investigate the magnetic behavior of 3d atoms in the  $ThMn_{12}$ -type structure, the structural and magnetic properties of  $Y(Al_{1-x}Fe_x)_{12}$  were studied by Mössbauer spectroscopy and magnetization measurements. The  $Y(Al_{1-x}Fe_x)_{12}$  intermetallic compounds crystallize in the  $ThMn_{12}$ -type structure for  $x$  in the range of 0.3–0.5. The results can be explained on the basis of the preferential atomic ordering observed in the ternary compounds. The compounds are ferromagnetic with Curie temperatures of 130, 170, and 280 K, respectively, for  $x$  values of 0.3, 0.4, and 0.5.

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## INTRODUCTION

We have investigated the structural and magnetic properties of  $Y(Mn_{1-x}Fe_x)_{12}$  which crystallizes in the  $ThMn_{12}$ -type structure [1]. The Y atoms occupy the 2a sites. The Fe and Mn atoms exhibit strong site preference with Mn favoring the 8i site and Fe the 8f site. A random, nearly stoichiometric distribution of the 3d atoms is observed on the 8j sites.

The magnetic behavior of  $Y(Mn_{1-x}Fe_x)_{12}$  is quite different from other Y-Mn-Fe systems [2,3,4]. Therefore, in an attempt to obtain more information concerning the behavior of Fe as its interactions with other magnetic atoms, i.e. Mn, are reduced, we have replaced Mn with non-magnetic Al. Accordingly, magnetic measurements and Mössbauer spectral studies of the ternary system  $Y(Al_{1-x}Fe_x)_{12}$  have been carried out. The results are compared with those reported for  $Y(Mn_{1-x}Fe_x)_{12}$ .

## EXPERIMENTAL

The samples were prepared by induction melting of the elements in a water-cooled copper boat under an argon atmosphere, and were then examined by x-ray diffraction. The magnetic measurements were made by using a vibrating sample magnetometer or a Faraday balance. The Mössbauer spectral measurements were obtained on a Ranger Instruments spectrometer which utilized a room temperature  $^{57}Co(Rh)$  source, calibrated with natural  $\alpha$ -iron foil [5].

## RESULTS AND DISCUSSION

Ternary compounds of  $Y(Al_{1-x}Fe_x)_{12}$  with  $x$  varying from 0.2 to 0.8, were studied by x-ray powder diffraction. Only lines of the  $ThMn_{12}$  structure were present for  $x=0.3, 0.4,$  and  $0.5$ .

The variation of the magnetization as a function of applied field at 4.2K for  $x=0.3, 0.4,$  and  $0.5$  is shown in Fig. 1. All these compositions are ferromagnetic. At  $H=12.5$  KOe, the magnetization of these samples attains values of 3.11 emu/g, 21.5 emu/g, and 50.5 emu/g, respectively. The corresponding Curie temperatures are 130, 170, and 280K. It should be mentioned that, although we find  $Y(Al_{0.7}Fe_{0.3})_{12}$  to be weakly ferromagnetic, Felner and Nowik report it to be antiferromagnetic [6].

The  $Y(Mn_{1-x}Fe_x)_{12}$  compounds with  $x \leq 0.67$  crystallize in the  $ThMn_{12}$  structure. In the range of  $x=0.1$  to  $x=0.5$ , they are antiferromagnetic (Fig. 2). When  $x$  is increased to 0.6, a ferromagnetic component is superposed onto the antiferromagnetic behavior.

The bulk magnetization of  $Y(Al_{0.7}Fe_{0.3})_{12}$  is quite low. On the basis of x-ray diffraction data for  $RFe_{11}Al_8$  [6] which show the Fe atoms occupying the 8f site, we conclude that the magnetic moment on the site is very weak ( $\sim 0.1 \mu_B$ /atom). This conclusion is consistent with the refinement of neutron diffraction results for  $Y(Mn_{1-x}Fe_x)_{12}$ , which indicates no magnetic moment on the 8f sites [1].

The room temperature Mössbauer spectra of  $Y(Al_{1-x}Fe_x)_{12}$  with  $x=0.3, 0.4,$  and  $0.5$  and  $Y(Mn_{1-x}Fe_x)_{12}$  with  $x=0.3$  and  $0.6$  indicate no long-range magnetic ordering, but do reveal different quadrupole interactions for different sites. Mössbauer spectra of  $Y(Al_{1-x}Fe_x)_{12}$  are shown in Fig. 3 and the resulting spectral parameters are summarized in Table I. The  $Y(Mn_{1-x}Fe_x)_{12}$  compounds have lower isomer shifts than Fe, hence a higher s-electron density at the nucleus. A similar effect has been reported for Mn-rich  $Y_6(Fe_{1-x}Mn_x)_{12}$  compounds and attributed to the higher electronegativity of iron relative to Mn and Y [4]. In contrast,  $Y(Al_{1-x}Fe_x)_{12}$  compounds exhibit higher isomer shifts than Fe and hence a lower s-electron density at the nucleus. The more symmetric 8f site (2/m) has a smaller quadrupole interaction than the 8j site (mm) which is of lower symmetry. The amount of iron on the 8i site is so low that the resulting parameters are probably less accurate, and therefore relative values may not be significant.

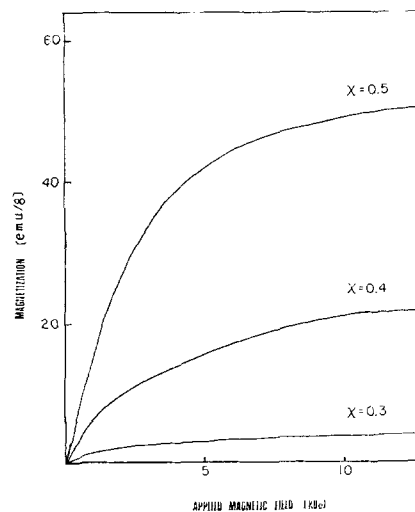


Fig. 1. Variation of the magnetization of  $Y(Al_{1-x}Fe_x)_{12}$  with field.  $T = 4.2K$ .

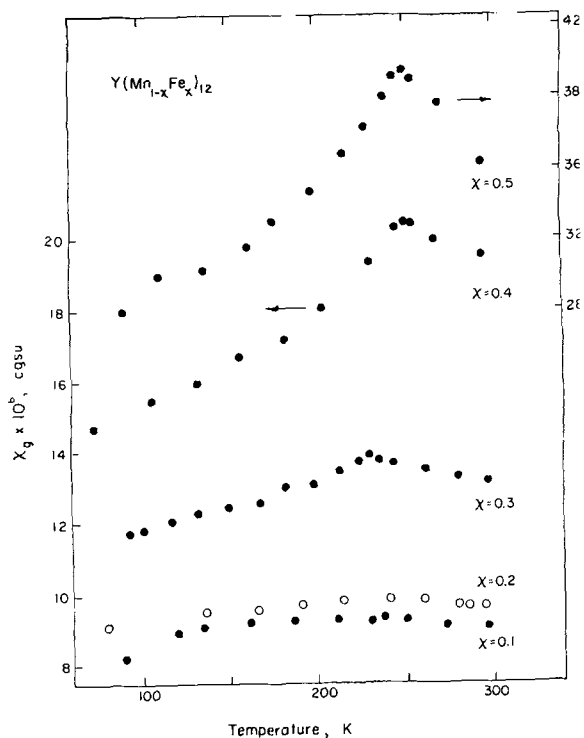


Fig. 2. Variation of the susceptibility with temperature of  $Y(Mn_{1-x}Fe_x)_{12}$ .

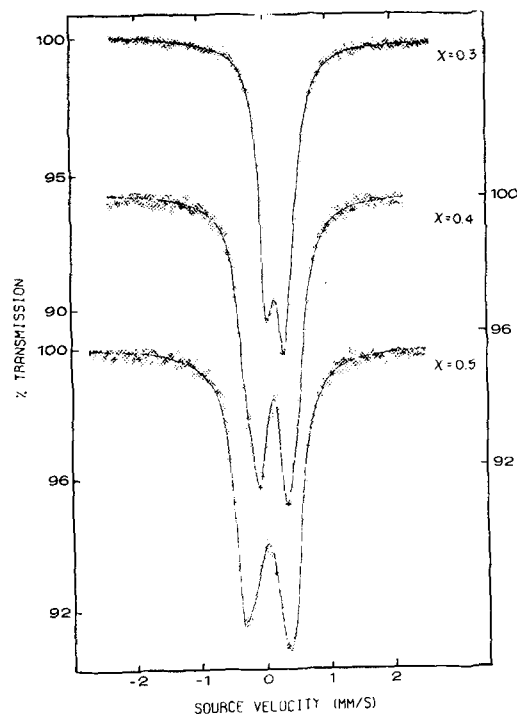


Fig. 3. Mössbauer spectra at  $Y(Al_{1-x}Fe_x)_{12}$  at room temperature.

TABLE I  
Mössbauer Effect Spectral Data<sup>a</sup>

Compound	T, K	i site (mm)				f site (2/m)				j site (mm)				$\chi^2$
		$\delta$	$\Delta EQ$	$\Gamma$	%A <sup>b</sup>	$\delta$	$\Delta EQ$	$\Gamma$	%A <sup>b</sup>	$\delta$	$\Delta EQ$	$\Gamma$	%A <sup>b</sup>	
$Y(Mn_{0.7}Fe_{0.3})_{12}$	297	-0.14	0.18	0.18	7.2	-0.20	0.53	0.29	58.0	-0.12	0.72	0.29	34.8	1.00
$Y(Mn_{0.4}Fe_{0.6})_{12}$	294	0.04	0.46	0.34	15.1	-0.10	0.58	0.30	46.5	-0.08	0.69	0.33	38.4	0.94
$Y(Al_{0.7}Fe_{0.3})_{12}$	296				0	0.19	0.29	0.31 <sup>c</sup>	100				0	1.08
					0	0.22	0.25	0.33	66.7	0.16	0.32	0.23	33.3	1.05
$Y(Al_{0.6}Fe_{0.4})_{12}$	296				0	0.14	0.41	0.33	66.7	0.11	0.77	0.31	33.3	1.07
					0	0.14	0.45	0.37	83.3	0.11	0.82	0.24	16.6	1.13
$Y(Al_{0.5}Fe_{0.5})_{12}$	293				0	0.10	0.46	0.45 <sup>c</sup>	66.7	0.09	0.81	0.27 <sup>c</sup>	33.3	1.11

<sup>a</sup> All data in mm/s relative to natural  $\alpha$ -iron foil.

<sup>b</sup> Relative areas are constrained to the values given

<sup>c</sup> Average of two slightly different linewidths.

Decreasing the Al content results in a larger  $\Delta EQ$ , which indicates an increasing distortion at both Fe sites.

We plan to carry out Mössbauer measurements on these systems at low temperature in order to determine whether long range magnetic ordering of the Fe is present on the 8f sites.

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