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P. Dalmas de Réotier, E. Gil, P. Vulliet, A. Yaouanc, P. Chaudouët, et al.. MÖSSBAUER INVESTIGATION OF IRON DOPED YBa₂Cu₃O_{7-x}. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-2203-C8-2204. 10.1051/jphyscol:19888989 . jpa-00229279

HAL Id: jpa-00229279

<https://hal.science/jpa-00229279>

Submitted on 4 Feb 2008

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MÖSSBAUER INVESTIGATION OF IRON DOPED $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$

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Abstract. – We have recorded ^{57}Fe Mössbauer spectra of $\text{YBa}_2(\text{Cu}_{1-y}\text{Fe}_y)_3\text{O}_{7-x}$ powder sample and uniaxially oriented powder for $0.01 \leq y \leq 0.1$ and $x \cong -0.2$ or $x \cong 0.6$. In the superconducting $x \cong 0$ compounds we see three subspectra for $y > 0.01$ and four subspectra for $y = 0.01$. These subspectra correspond to different oxygen configurations around the iron atoms. From the oriented $\text{YBa}_2(\text{Cu}_{0.94}\text{Fe}_{0.06})_3\text{O}_{7.2}$ and $\text{YBa}_2(\text{Cu}_{0.9}\text{Fe}_{0.1})_3\text{O}_{6.4}$ compounds we deduce that more than 90 % iron substitutes Cu(1) site. The iron magnetic moments order antiferromagnetically at $\cong 18$ K and $\cong 1.5$ K for the $x = -0.2$, $y = 0.06$ and $x = 0$, $y = 0.01$ compounds respectively.

Xiao *et al.* [1] have studied the effect of small amounts of transition metal atoms on the superconducting temperature of $\text{YBa}_2\text{Cu}_3\text{O}_7$ samples. Surprisingly, they found that superconductivity is not suppressed even for reasonably high iron concentration. In usual superconductors a small amount of magnetic impurity destroys superconductivity. In order to understand this surprising result, microscopic information on the iron atom localization and valency is essential. ^{57}Fe Mössbauer is an ideal tool for that purpose.

Many papers have reported ^{57}Fe Mössbauer results but only recently detailed studies have been published [2]. Previously, we have shown directly from measurements on $\text{YBa}_2(\text{Cu}_{0.94}\text{Fe}_{0.06})_3\text{O}_{7.2}$ oriented powder that iron substitutes for Cu(1) at least for the main two sites because the principal axis of the electric field gradient is in the $a-b$ plane [3]. Due to the weak intensity of the site with the quadrupole splitting $|\Delta| = 0.52$ mm/s, it is not possible to obtain from the fit the orientation of the main axis of the electric field gradient at that site. Here we report results obtained on powder samples with $y = 0.10$, 0.06 , 0.02 , 0.01 for $x \cong 0$ and $x \cong 0.6$. In addition, a measurement at room temperature on oriented powder of $\text{YBa}_2(\text{Cu}_{0.9}\text{Fe}_{0.1})_3\text{O}_{6.4}$ has been performed which confirms that the iron atoms are in the Cu(1) site.

We have measured the temperature dependence of the recoil-free fraction for the oriented powder and

powder samples with $y = 0.06$ and $x \cong -0.2$. The two set of data can be described by the same Debye temperature of 420 (30) K. This result confirms that the quadrupole doublets are symmetric in the powder.

In the $y = 0.01$, $x \cong 0$ sample four quadrupole doublets are present. This is in contrast to the other $x \cong -0.2$ samples where only three doublets are seen [3]. In this sample, the quadrupole splittings are temperature independent up to $\cong 200$ K. From this temperature to 310 K they decrease by $\cong 5$ %. For the other samples, the quadrupole splittings are temperature independent in the whole temperature range. In the table I we present the hyperfine parameters for the $y = 0.01$, $x \cong 0$ sample at 77 K. We do not give the sign of the quadrupole splitting of doublet 4 because we have not performed measurements on an 1 % iron doped oriented sample. The sign for doublet 1 and 3 is deduced from the measurements on the 6 % sample. For the first three doublets the parameters are about the same for all our $x \cong 0$ samples except the intensity of doublet 1 which is larger by $\cong 25$ % for $y = 0.10$ and the intensity of doublet 3 which decreases by $\cong 50$ % for $y = 0.10$. In this last comparison, doublet 3 and 4 are considered together. About 80 % of the spectra of the $x \cong 0.6$ samples can be described by the third doublet of the table. The direction of the main axis of the electric field gradient is definitively in the $a-b$ plane and is positive as in the $x \cong 0$ compound.

Table I. – Relative intensity (in %) and hyperfine parameters (in mm/s) for each doublet in $\text{YBa}_2(\text{Cu}_{0.99}\text{Fe}_{0.01})_3\text{O}_7$ at 77 K.

	Db. 1	Db. 2	Db. 3	Db. 4
Intensity	62	8	15	15
Quadrupole splitting	+1.03	± 0.55	+2.04	± 1.55
Isomer shift	+0.07	+0.46	+0.10	–0.03
line width (FWHM)	0.48	0.25	0.24	0.25

In the figure 1, we present the spectra obtained at 4.2 K for the oriented powder (c axis parallel to the γ ray) and the powder of $\text{YBa}_2(\text{Cu}_{0.94}\text{Fe}_{0.06})_3\text{O}_{7.2}$. Measurements below 4.2 K on these samples give the same results. Except for the two thin central lines the other lines have about the same intensity in the two spectra. In addition the lines are wide. These results show that the magnetic moments which correspond to these lines are in a spin glass-like state. These moments correspond to a hyperfine field of 250 kOe. The lines at $\cong -7$ mm/s and $\cong +7.5$ mm/s correspond to a hyperfine field of $\cong 450$ kOe and originate from the iron of the second doublet. The two central lines are probably due to iron with a small hyperfine field: $\cong 100$ kOe.

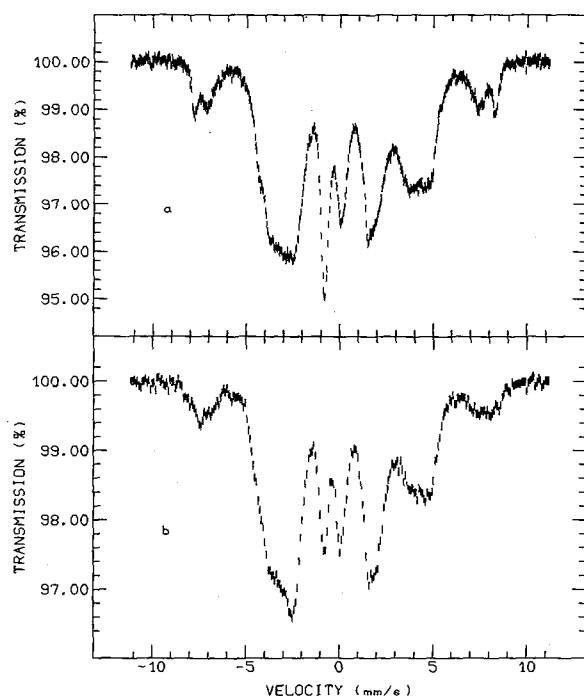


Fig. 1. - ^{57}Fe Mössbauer spectra of $\text{YBa}_2(\text{Cu}_{0.94}\text{Fe}_{0.06})\text{O}_7$ at 4.2 K: a: powder; b: oriented powder.

All these data show that iron substitutes Cu(1) site with different oxygen configurations. The only difference between the samples (except for the $y = 0.01$ sample) is the intensity of the different configurations. The fourth doublet of the $y = 0.01$ sample probably transform to the third doublet for higher iron concentration because of the orthorhombic-tetragonal crystallographic transformation. More work is needed to definitely associate the different doublets to an oxygen configuration and to an iron valency. Still it is probable that doublet 2 because of its isomer shift, its small quadrupole splitting and its large hyperfine field is due to Fe^{3+} with a spin $S = 5/2$ and with six oxygen nearest neighbours. Because of the hyperfine parameters the other doublets can only be due either to Fe^{3+} with $S = 3/2$ or Fe^{4+} with $S = 1$. From the value of the isomer shift for doublet 1, the valency Fe^{4+} is maybe more probable [6]. The oxygen environment corresponds probably to a square planar pyramidal for doublet 1 and to a four fold coordination for doublet 3 and doublet 4 as determined by a comparison with a point charge calculation. Our interpretation is supported by the diffraction measurements of reference [4] but are at variance to the diffraction results of reference [5].

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