Physica C 162–164 (1989) 989–990
North-Holland

LOCAL MAGNETIC FIELDS IN THE Cu SITES OF $YBa_2Cu_{3-x}Fe_xO_y$ DETECTED BY MÖSSBAUER SPECTROSCOPY

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The temperature dependence of the Mössbauer parameters of the spectra of an $YBa_2Cu_{3-x}Fe_xO_y$ superconducting sample, with $x = 0.125$, together with a strong temperature dependent asymmetry in one of the three observed quadrupole doublets, suggests the existance of a small magnetic field in the positions of the Fe atoms, which are assumed to be only the Cu(1) sites of the 1-2-3 structure.

Mössbauer spectroscopy has proven to be a useful tool to investigate the local surroundings of the Cu sites of superconducting 1-2-3 systems. Actually, it is now recognized that Fe atoms substitute preferentially in the Cu(1) sites of the structure (at least for small Fe concentrations)[1,2] and that the information about the local environment of these sites obtained with Mössbauer spectrocopy, can give some clues about the influence of the Cu(1)-O chain in the superconducting mechanism of these systems[3]. Unfortunately, only few systematic temperature analysis have been made of the behaviour of the Mössbauer parameters around T_c for these systems at different Fe concentrations.

In the present paper we report results obtained from a $YBa_2Cu_{3-x}Fe_xO_y$ superconducting sample, with $x = 0.125$, using a low velocity scan ($\sim \pm 1.8 \frac{mm}{s}$) at several temperatures, ranging from 11 K to room temperature.

The sample was prepared by solid state reaction using natural Fe_2O_3 and the Mössbauer spectra were obtained with a constant acceleration spectrometer in transmission geometry. All the spectra showed two prominent doublets ($\Delta Q_A \sim 2.0 \frac{mm}{s}$ and $\Delta Q_B \sim 0.6 \frac{mm}{s}$) and a third doublet ($\Delta Q_C \sim 0.6 \frac{mm}{s}$) of smaller intensity. Fig. 1 shows some of the obtained spectra and Table 1 summarizes the temperature dependence of the parameters of each doublets, for all the temperatures used in our study. As can be seen in Fig. 1, the asymmetries in the quadrupole doublets vary with temperature.

The observed temperature dependent asymmetries can not be explained by a Kargyagin-Goldanskii effect, nor by a residual crystallite orientation in the powdered sample. Rather, we propose that they are due to com-

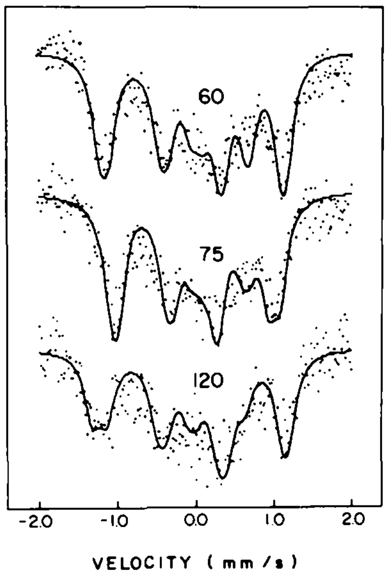

FIGURE 1
Mössbauer spectra at different temperatures.

*This work was partially supported by the PUSCATT and PSPA, UNAM, and by CONACyT, México.

0921-4534/89/$03.50

T(K)	IS_A $\pm.01$	ΔQ_A $\pm.01$	θ_A	A_A 10^{-3}	IS_B $\pm.01$	ΔQ_B $\pm.01$	A_B 10^{-3}	IS_C $\pm.02$	ΔQ_C $\pm.02$	θ_C	A_C 10^{-3}
11	.16	1.97	90	1.09	.11	.59	.87	.46	.53	90	.60
45	.17	1.95	90	1.10	.14	.60	.80	.47	.52	65	.65
60	.16	1.94	90	1.00	.15	.61	.86	.49	.59	40	.65
75	.16	1.73	42	1.04	.15	.50	.85	.46	.56	65	.50
90	.16	1.68	72	0.96	.10	.53	.85	.38	.45	30	.60
120	.15	1.90	90	0.57	.13	.60	.53	.39	.49	30	.35
140	.15	1.95	50	0.92	.13	.59	.80	.45	.55	30	.50
300	.06	1.92	65	0.79	.14	.54	.82	.43	.47	30	.35

TABLE 1

In all cases, the magnitude of the magnetic field is 5.7 kOe, $\theta_B = 90, \eta_A = \eta_B \simeq 0.6$ and $\eta_C = 0$ and $\Phi_A = \Phi_B = \Phi_C = 0$, except for T = 120 K, where $\Phi_A = 90$.

bined electric and magnetic interactions in the Cu sites where the Fe atoms go to, and that these are only the Cu(1) sites of the structure, surrounded by two, four and six oxygen atoms. The reason for this last assumption is based on the fact that when a superconducting sample is heated in Ar atmosphere[4] or in vacuum[5], there is a drastic reduction of the absorption of the central doublets (B and C) and a concomitant enhacement of the relative absorption of the external one (A). This experimental fact can be understood by the variation of the surroundings in the Cu sites due to the well known O(4) and O(5) movility around 800 K, and it is incompatible with the assumption of Cu(2) substitution by Fe, since in that case one should not expect a dramatic effect with temperature in the absorption of the corresponding doublet.

The spectra were fitted using a Hamiltonian that includes an electric field gradient and a magnetic field, using Kündig's graphs as a guide to fix the initial values of the different parameters (the solid line in the spectra of Fig. 1 represent the results of the fitting process). It is particularly important to fix the magnitude of the magnetic field and this was done choosing the largest field magnitude consistent with experimental data associated with doublet A, since the variations in its asymmetry are most apparent. Once this value is fixed, the other two doublets can be adjusted.

As a result of the fitting process, we conclude that a) a change in the orientation of the assumed magnetic field with respect to the electric field gradient principal axis can reproduce the experimental data fairly accurately, meaning that the magnetic effect is exclusively responsible for the asymmetry of the doublets; b) there are drastic changes in the magnetic configuration between 60 K and 100 K (see the angle θ variations in Table 1); c) as reported before[6], it was confirmed that the quadrupole splittings and isomer shifts of the doublets are affected around the same temperature range.

The existence of small magnetic fields could be due to the incorporation of magnetic atoms in the structure, or to magnetic interactions already existing in the pure material[7]. In any case, the confirmation of our assumption would represent another piece of evidence of the apparent interplay between magnetic order and superconductivity.

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