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ANGULAR CORRELATION STUDY OF HYPERFINE INTERACTIONS IN $YBa_2Cu_3O_y$**

by

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ABSTRACT

Angular Correlation experiments were performed on Y-Ba-Cu-O structures, oxygenated and argonized phases, in the temperature range 77K-600K. The displayed nuclear quadrupole interactions (NQI) lead to: (i) different lattice sites; (ii) remarkable difference between oxigenated and argonized phases.

Key-words: Angular correlation; Hyperfine interactions; Y-Ba-Cu-O structures.

1 INTRODUCTION

Since the discovery of high T_c superconductivity in Y-Ba-Cu-0 much effort has been made to characterize the structure and composition of both phases, normal and superconducting (1); they show, for instance, the existence of two copper sites: Cu1 has a square planar coordination due to the presence of two oxygen vacancies in the $\vec{a}$ axis, whereas Cu2 has a tetragonal pyramidal coordination due to an oxygen vacancy in the $\vec{c}$ axis. Additional information, with extension to dynamical effects, as those obtained from hyperfine interactions (HFI), revealed by local spectrocopies such as Perturbed Angular Correlations (PAC), may be of great interest since they reflect the microscopic charge distribution at the probe nucleus. We have investigated by (PAC), in it's time differential mode, above and below T_c, in oxygenated as well as argonized samples, the electric field gradients (EFG) at the site of dilute Cd^{111} impurities ($\sim 10^{-5}$ at.%) in Y-Ba-Cu-0.

2 EXPERIMENTAL DETAILS AND RESULTS

The measurements were carried out with the (172-247) keV cascade of Cd^{111} which is populated by the EC decay of the 2.8 days In^{111} isotope. For the measurements we used a four detector apparatus, each detector being 90^0 apart from the other. The normalized data were least-square fitted with the function

$$G_{kk}(t) = \sum_{n=0} \sigma_{Kn} \cos(\omega_n t)^{(2)} \quad , \quad \text{with } K = 2 \qquad (1)$$

appropriate for a static quadrupole interaction in a polycrystaline source with a nuclear spin $I = 5/2$[2]. The finite time resolution was about 4.0 nsec. Polycristaline samples (named Sample I and Sample II) of Y-Ba-Cu-O were prepared[3] from a mixture of pure Y_2O_3, $BaCO_3$ and CuO; the activity was introduced in the sample during sinterization. The argonization was done at 500C, under argon flux, during 2hs. From the temperature dependence of the magnetic susceptibility, $\chi_g = M_g/H$, the values of T_c (here defined as the temperature at which the susceptibility crosses the $\chi_g = 0$ line) were derived[4]. (PAC) measured with these samples were characterized by non-axially symmetric pure quadrupole interactions related to two sites in Sample II and to three sites in Sample I. X-ray analysis yielded ortorhombic structure to the oxigenated samples and tetragonal structure to the argonized ones. In all samples was detected the presence of an $\sim$ 5% admixture of In_2O_3, as a precipitated phase, which d'ont interfieres in the measurements as far it don't includes any of the Y-Ba-Cu atoms in it's structure. Fig. 1 show (PAC) spectra obtained with such samples in various temperatures. The values of the quadrupole frequencies (QF) of the (EFG), of the assymetry coefficients η, as well as of some of the fit parameters, are displayed in Table I.

3 DISCUSSION

The most important features of the (HFI) measured in samples I and II are: (i) quadrupole frequencies (QF) of Samples I are quite similar to those of Sample II, beside a third (QF) which appears in Sample I, inexistent in Sample II; (ii) small variation of (QF) with temperature in both samples; (ii) $\eta = 0$ for the 77K Sample II measurement; (iv) remarkable difference between oxigenated and argonized samples spectra.

Concerning Sample II, the two measured (QF), beside the In_2O_3 assigned frequency, are quite close each other and with the lower one, at 296K, at a site rate about five times higher than the second one: this site rate discrepancy seems to avoid the possibility of assigning each of the (QF) to the two different copper sites, which are known to appear at a site rate 2:1 in the Y-Ba-Cu-O structure. By other side, (EFG) calculations performed using a point-charge model(*) displayed a much higher (QF) intensity ratio than the ω^1/ω^2 = .85 we obtained. At this moment we could like to advance that we are dealing with one (QF) related to only one probe-site, probably with slight site distortions and/or oxygen content apart from $\delta = 7$. It remains to clear out the nature of this site. In this sense, the argonized sample displays one site with only one (QF), and, as the Cu oxygen environment content is highly changeable upon argon substitution, we would be

(*) S. Vries - Private communication.

tempted to say that the site we are dealing with should be the Cu1 site. A remarkable figure concerned with the 77K result is, beside the equalization of the two (QF), even with different sites assignments, that one of the sites η drops to zero ($V_{xx}=V_{yy}$), configurating an axial simmetry, and this, even cautiously, may be tributed to a higher occupancy of the vacancies around Cu1, which are known to exist, or by a redistribution of density changes below T_c or/and by a higher moving of the 0_2 themselves, with a consequent simmetry improving (tetrahedral - octahedral). As a counterpoint, we will not extend about Sample I, as far as we may notice that the corresponding (QF) results are quite similar to those of Sample II, beside the third (QF) that, we believe, may be due to a crystaline local misformation. The above results seems to confirm that the investigation of (HFI) in the Y-Ba-Cu-0 compounds can supplement structural, as well as dynamical, results obtained by other techniques.

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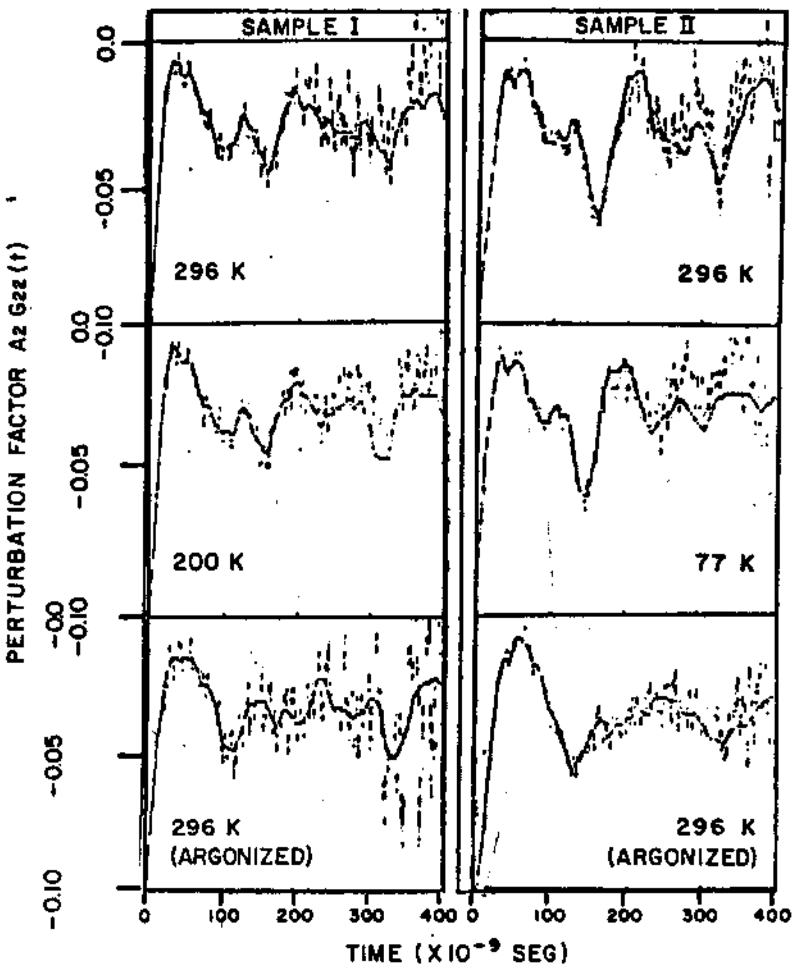

Figure 1

Fig. 1 - PAC spectra of YBaCuO(Cd^{111}).

TABLE I. PAC measured parameters for $YBa_2Cu_3O_y$ doped with Cd^{111}: S^i (site fractions in %); ω^i (quadrupole frequencies in Mrad); η^i (assymetry coefficients); δ^i (quadrupole frequencies distributions in %); V_{zz} (electric field gradients in 10^{17} Volt/cm^2).

SAMPLE I															
T(K)	S^1	ω^1	η^1	δ^1	V^1_{zz}	S^2	ω^2	η^2	δ^2	V^2_{zz}	S^3	ω^3	η^3	δ^3	V^3_{zz}
296	36.63	6.2	.31	1.0	5.053	23.16	7.0	.40	5.0	2.317	44.21	9.1	.36	11.0	3.014
200	28.42	6.3	.23	0.0	2.085	27.37	6.8	.49	4.0	2.248	43.16	8.7	.39	8.0	2.506
296 argon.	33.33	5.7	.36	2.0	1.884	18.75	7.8	.39	0.0	2.581	47.92	9.3	0.0	11.0	3.077
SAMPLE II															
296	83.52	6.0	.34	4.0	1.987	16.48	6.7	.58	1.0	2.217					
77	36.66	6.5	0.0	4.0	2.154	63.33	6.5	.47	7.0	2.157					
296 argon.	100.0	4.6	.61	13.0	1.519										

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