Theory of muon resonance of level crossing in a superconducting $YBa_2Cu_3O_{7-x}$ ceramic

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A strong angular dependence of resonance magnetic fields should be observed in $YBa_2Cu_3O_{7-x}$ ceramics. The rate of decay of the polarization at a resonance depends strongly on the resonance field. This dependence changes qualitatively as a result of reversal of the sign of the quadrupole interaction constant and for different pores containing a muon. The angular dependences of the resonance magnetic fields change qualitatively as a result of a change from 1 to 1/2 in the parameter η representing the symmetry of the electric field gradient.

The muon method is used widely in various magnetic measurements on $YBa_2Cu_3O_{7-x}$ (1–2–3) ceramics. However, in the interpretation of many of them (for example, in the case of the data on antiferromagnetism) it is desirable to know the position of a muon in the lattice. Conventional methods for determination of this position by relaxation in zero and transverse magnetic fields may lead to indeterminacies associated with the fact that relaxation of 1–2–3 ceramics may be governed not only by nuclear spins, but also by paramagnetism. It would therefore be interesting to use the resonance method to identify a pore containing a muon.

The muon level-crossing resonance predicted by Abragam[1] and first discovered in copper[2] should have a number of special features in the case of 1–2–3 ceramics. This is due to the fact that, in principle, there are two possible positions of a muon[3] in a 1–2–3 ceramic and for both these positions there is a strong electric field gradient (EFG) at the copper nuclei closest to the muon, so that the NQR frequencies amount to ~20 and ~30 MHz (Ref. 4); moreover, there are only two copper atoms near the muon.

The positions of copper atoms relative to a muon vary with the nature of the pore and, therefore, we hope that the resonance patterns for different pores would be different. A muon is a polarized particle so that the angular dependences of muon resonances in single crystals should be stronger than NQR. Hence there is hope that additional information can be obtained on the symmetry parameter η of the EFGs. Although a muon itself also creates an EFG, it follows from the data on pure copper that it corresponds to frequencies ~1 MHz, which are an order of magnitude lower than the frequencies associated with the lattice of the 1–2–3 ceramics themselves. Therefore, the indeterminacies of the parameters of the EFG because of lattice deformation by an interstitial muon should be slight. Moreover, we shall see later that strong deformations may appear in the course of measurements.

Since there are only two copper nuclei (which, moreover, have small spins) near a muon in a 1–2–3 ceramic, it is possible to carry out precision calculations on a computer.

A muon in the perovskite lattice may occupy, in principle, two positions[3]: either between Cu II atoms in a plane perpendicular to the c axis and passing through a rare-earth atom (pore II) or in a plane of Cu I atoms along the edge between two Cu I atoms (pore I). The experiments reported in Ref. 3 suggest that a muon is located near Cu I, but there are still some problems associated with the possible superposition of the paramagnetic relaxation effects and of relaxation due to the nearest nuclei.

In the case of a sample of a 1–2–3 ceramic containing just one Cu isotope, the Hamiltonian of the interaction is

$$\mathcal{H}=\hbar\left\{-\gamma_\mu\hat{\mathbf{S}}_\mu\mathbf{H}-\sum_{l=1,2}\gamma_{Cu}\hat{\mathbf{I}}_l\mathbf{H}\right\}+\mathcal{H}_Q+\mathcal{H}_{dip}. \quad (1)$$

Here, γ_μ and γ_{Cu} are the gyromagnetic ratios of a muon and a Cu nucleus; $\mathbf{H}$ is an external magnetic field parallel to the initial polarization of the muon; $\hat{\mathbf{I}}$ is the spin operator for l th copper nucleus; $\hat{\mathbf{S}}_\mu$ is the muon spin operator; $\mathcal{H}_{dip}$ is the part of the Hamiltonian associated with the dipole–dipole interaction:

$$\mathcal{H}_{dip}=\sum_{l=1,2}\frac{\hbar^2\gamma_\mu\gamma_{Cu}}{R_l^3}[(\hat{\mathbf{I}}_l\hat{\mathbf{S}}_\mu)-3(\hat{\mathbf{I}}_l\mathbf{n}_l)(\hat{\mathbf{S}}_\mu\mathbf{n}_l)], \quad (2)$$

where $\mathcal{H}_Q$ is the quadrupole part of the Hamiltonian which in the system of the principal axes of the EFG ellipsoid is

$$\mathcal{H}_Q=\pi\nu_Q\hbar\sum_{l=1,2}[(\hat{I}_l^z)^2+\eta(\hat{I}_l^x)^2-\frac{1}{3}I_l(I_l+1)(1+\eta)]. \quad (3)$$

Here, ν_Q is the quadrupole interaction constant. In the case of the $I=3/2$ spin and $\eta=1$ or $\eta=0$ the constant ν_Q is equal to the NQR frequency. The principal axes are distributed as follows in the pore I (Refs. 5 and 6): z_0 is along the direction of the Cu I–O–Cu I chain, y_0 is along the c axis of the crystal, and x_0 coincides with the direction from the muon to the Cu I atom.

It is known from the NQR measurements reported in Refs. 5 and 6 that the symmetry parameter is $\eta\approx0.9$ for the Cu I nuclei. Since we are ignoring the influence of the muon on the electric field, we can assume without further loss in precision that $\eta=1$.

In the pore II, located in a superconducting plane, the z_0 axis is directed along the c axis and coincides with the muon–nucleus direction,[5,6] and the parameter η for the pore II (at the Cu II nuclei) is approximately zero.

In a coordinate system oriented in an arbitrary manner relative to the principal axes, the quadrupole part of the Hamiltonian is

$$\mathcal{H}_Q=\hbar\pi\nu_Q\sum_{l=1,2}\{(\hat{I}_l^z\cos\theta+\hat{I}_l^x\sin\theta\sin\varphi+\hat{I}_l^y\sin\theta\cos\varphi)$$
$$+\eta[\hat{I}_l^x(\cos\psi\cos\varphi-\cos\theta\sin\psi\sin\varphi)+\hat{I}_l^y(-\cos\psi\sin\varphi-\cos\theta\sin\psi\cos\varphi)+\hat{I}_l^z\sin\theta\sin\psi]^2\}, \quad (4)$$

where θ, φ, and ψ are the Euler angles (standard notation).

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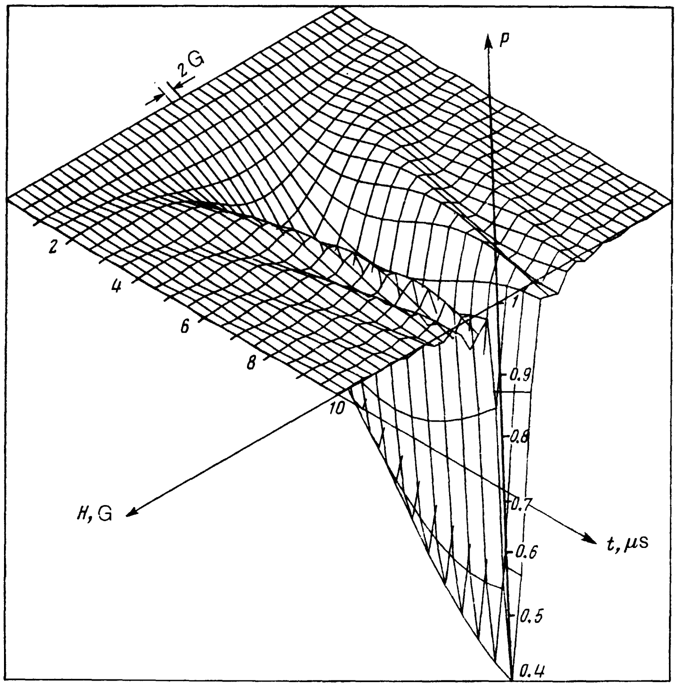

FIG. 1. Polarization of a muon plotted as a function of time and of the magnetic field in the pore I for a resonance at $H_{res} = 1500$ G.

The muon–nucleus direction can be desired as follows in terms of the Euler angles: in the pore I, we have

$$n_x = \cos\psi\cos\varphi - \cos\theta\sin\psi\sin\varphi,$$

$$n_y = -\cos\psi\cos\varphi - \cos\theta\sin\psi\cos\varphi, \quad n_z = \sin\theta\sin\psi, \tag{5}$$

and in the pore II

$$n_x = \sin\theta\sin\varphi, \quad n_y = \sin\theta\cos\varphi, \quad n_z = \cos\theta. \tag{6}$$

The muon polarization is

$$P(t) = \sum_k \mathrm{Tr}[\Psi^* \exp(-i\omega_k t) S_\mu^z \exp(i\omega_k t)\Psi_0]\frac{1}{N}, \tag{7}$$

where ψ_0 is the function of the initial state allowing for the initial polarization of the muon and N is the normalization factor. The trace (Tr) is taken over all the initial states of the nuclear spins and the sum over k means summing over the frequencies.

We simplified the program part by increasing the distance between the muon and one of the nuclei to 3×10^{-5} in relative units. We investigated several variants: $\eta = 1$ (which corresponds to the pore I), $\eta = 0$ for the pore II, and also the case $\eta = 1/2$ in order to check the sensitivity of the results to the deformation of the lattice by the muon. In addition to diagonalization of the matrices, we checked the calculations by the method of time-dependent perturbations involving 120 orders for the situation when $\nu_\alpha \leqslant$ MHz. The agreement between the two sets of results obtained by different methods guaranteed freedom of program errors.

There is a certain self-similarity between the resonance field and the quadrupole interaction constant. Let us assume that, for example, only the quantity $\partial^2 V/\partial z_0^2$ differs from zero i.e., that there is a specific axis z_0 if the magnetic field is directed along a different direction at an angle θ, so that the nuclear levels depend not only on the field but also on the angle θ. The difference between the energies of two levels should be

$$\Delta_{ik} = \pm 2\pi\nu_Q\hbar + f_{ik}(\theta, H/\nu_Q)H. \tag{8}$$

At a resonance we should have

$$\pm 2\pi\hbar\nu_Q + f_{ik}(\theta, H/\nu_Q)H = \mu_\mu H, \tag{9}$$

i.e., the resonance field is proportional to the quadrupole interaction constant, since the ratio of the resonance field to this constant is described by an equation which depends only on the angle and on the world constants which are $\hbar$ and the magnetic moment of the muon μ_μ:

$$\frac{H_{res}}{\nu_Q} = \frac{\pm 2\pi\hbar}{\mu_\mu - f_{ik}(\theta, H_{res}/\nu_Q)}. \tag{10}$$

If beside $\partial^2 V/\partial z_0^2$, the derivative $\partial^2 V/\partial x_0^2$ also differs from zero, we find that f_{ik} in Eq. (10) depend also on the second angle, but the nature of the above expression is not affected. Therefore, an increase in the quadrupole transition frequen-

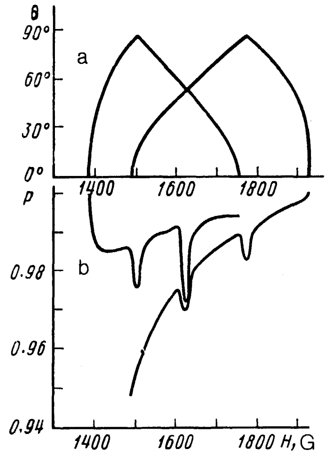

FIG. 2. Dependences of the resonance field in the pore I on the angle behind the c axis and the magnetic field (a) and the muon polarization at $t = 2\ \mu$s plotted as a function of the resonance field under resonance conditions (b).

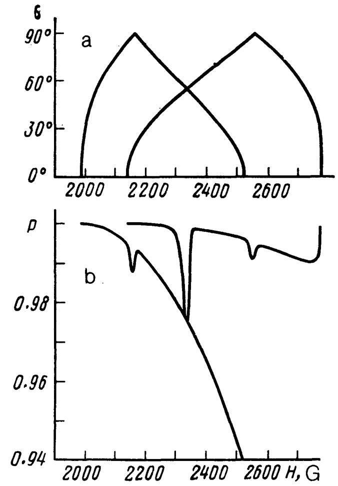

FIG. 3. Same as in Fig. 2, but for the pore II.

cy in a constant geometry should result in a proportional increase in the magnetic field, apart from the width governed by the dipole–dipole interaction. It also follows from Eq. (10) that reversal of the sign of the quadrupole interaction does not alter the position of a resonance, but it is now due to different transitions. It should be noted that a Hamiltonian of the $\hat{I}_{z_0}^2 + \hat{I}_{x_0}^2$ type expressed in terms of other axes is equivalent to $-\hat{I}_{z_1}^2$, i.e., it seems to correspond to a negative quadrupole interaction constant. These qualitative ideas make it much easier to find the resonances of ^{65}Cu from the well-known resonances of ^{63}Cu; moreover, the resonances in the pore II can be found from the resonances in the pore I: in the latter case we need to allow for the change in the quadrupole interaction constant, whereas a change in the distance between the muon and the copper nuclei alters only the degree of depolarization at a resonance.

Figure 1 shows a characteristic dependence of the resonance field on the applied magnetic field and on time. It is clear from this figure that at $t = 2\,\mu s$ the half-height width of a resonance is 27 G, whereas at $t = 10\,\mu s$ it is only 2 G, i.e., a strong narrowing of a resonance occurs with time. Figure 2 shows the dependences of the resonance field for ^{63}Cu on the angle between the magnetic field and the crystal c axis for the pore I and the dependence of the polarization on the resonance field at $t = 2\,\mu s$ at resonance. Figure 2 shows clearly the angles at which a resonance can be observed reliably.

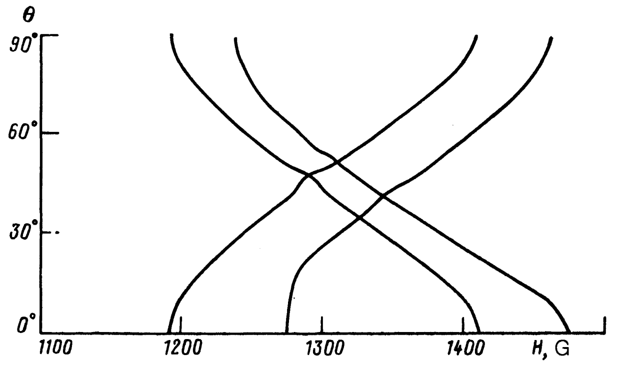

FIG. 4. Dependences of the resonance fields on the angle between the c axis and the magnetic field when the symmetry parameter is $\eta = 1/2$.

Similar dependences for the pore II are given in Fig. 3. The dependences of the resonance power (of the polarization at $t = 2\,\mu s$) are now qualitatively different. This is because the greatest contribution to the resonance comes from transitions which do not alter the sum of the projections of the muon and nuclear spins. This happens when the change in the projection of the nuclear spin is alterered by 1. In general, we can expect $3/2 \to 1/2$, $3/2 \to -1/2$, $-3/2 \to -1/2$, $-3/2 \to 1/2$, or $1/2 \to 3/2$, $-1/2 \to 3/2$, $-1/2 \to -3/2$, $1/2 \to -3/2$ transitions. Depending on the sign of the quadrupole interaction constant, one of these possibilities applies. The initial muon polarization creates a strong difference within these variants. Strictly speaking, this is justified only for the first orders of secular perturbation theory treatments. In reality the process is governed by thousand-fold orders, but the picture is qualitatively the same.

The power of a resonance depends also on the angle between the field and the muon–nucleus direction. This dependence is weak and the resonance appears more strongly if this angle is 90°. A strong dependence of the resonance power on the sign of the constant suggests that the resonance position may be sensitive to a change in η. This was checked by calculating the $\eta = 1/2$ case for the pore I. Then, the quadrupole interaction constant was corrected so as to retain the initial NQR frequency. We can see from Fig. 4 that the angular dependence of the resonance fields is not affected qualitatively. It follows that if a muon deforms strongly the lattice, i.e., if it creates a large gradient along the c axis (i.e., if the parameter η decreases), then this should be easily detectable in experiments. Therefore, the problem of the degree of influence of a muon on the lattice can be solved experimentally.

An analysis of the results obtained shows that in the case of polycrystalline samples the resonance effects are strongly averaged out, since the width of a resonance is only 27 G and the positions of the resonances vary by hundreds of gauss. Therefore, we can obtain additional information on the symmetry parameter of the EFG only if we use single crystals.

It therefore follows that the muon resonance of level crossing in single crystals should become a very sensitive instrument for the determination of the EFG and of its symmetry, and in particular it is very sensitive to the type of a pore in which a muon is located.

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