89Y NMR line splitting in the high Tc superconductor YBa2Cu3O7

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The $^{89}$Y nuclear resonance line in the superconducting compound YBa$_2$Cu$_3$O$_7$ has been measured as a function of temperature at a frequency of 10 MHz. The room temperature single line is found to be split in two lines at 100K. The implications of this result are discussed.

The present high $T_c$ superconducting oxides are either based on doped La$_2$CuO$_4$ or on YBa$_2$Cu$_3$O$_7$ (YBCUO). In the first group with superconducting transition temperatures of around 40 K, quadrupole resonance on the rare earth (RE) nucleus has revealed the antiferromagnetic order in these materials [1,2]. In performing a resonance study on the RE-nucleus in the orthorhombic or tetragonal phases of YBCUO the following should be kept in mind: the crystal structure implies a cancellation of the fields produced by oriented copper moments at the RE-site; furthermore the electron density at the RE-site is expected [3] and observed [4] to be low. From these considerations Cu as resonance probe would seem more favourable, but the resonance line was found to be extremely broad, apparently due to the quadrupolar momentum of the \(I=3/2\) Cu nucleus. Doping of the copper site by a \(I=1/2\) nucleus is limited to iron, and, because of its low nuclear moment and low natural abundance of $^{57}$Fe not feasible. Oxygen replacement by fluorine has so far not produced stable compounds with reproducible transition temperatures. Hence, to get microscopic information via NMR one is limited to $^{89}$Y.

In this Communication we report the experimental results of a line width study on $^{89}$Y in YBCUO. The onset of diamagnetism in our sample, as determined by magnetic susceptibility was found to be at 90.2 K with a reflection point at 70 K [5]. The NMR measurements were performed in a magnetic field of 4.7 T (9.798 MHz) in the normal state of the material.

Figure 1 shows the Fourier transform of the NMR-FID as obtained at 298 K and 100 K. All data were taken using a pulse sequence consisting of a comb of 90° pulses (20 µs) followed by a 90° probing pulse with a dead time of 120 µs. At both temperatures checks were made on spurious signals by the application of a saturating pulse sequence. Also, the intensity was as expected from a calibration of the set-up, showing that no traces of other phases were the origin of the signal. At room temperature the single line has a width of 2kHz (about 1 mT), an order of magnitude more than the magnetic field inhomogeneity and a small positive shift of ~2 kHz. The relaxation time $T_{1n}$ is found to be ~12 s. At 100 K the line is split (\(\Delta v = 2 \text{kHz}\)). The relaxation time is roughly 20 s.

The room temperature relaxation time of 12 s and the relative line shift of 0.02 % can be related by the Korringa relation:

$$T_{1n}(\Delta H/H)^2 = (h/4\pi kT)(\gamma_e^2/\gamma_n^2),$$

with $\gamma_e$ and $\gamma_n$ being the electronic and nuclear gyromagnetic ratio's. This shows that although the line shift is small and the relaxation time quite long, the conduction electron density at the Y-site is still responsible for the NMR properties. We like to mention at this point...
that we were not able to observe $^{169}$Tm and $^{171}$Yb resonances in the corresponding (Tm/Yb)BaCuO compounds under the same experimental conditions (despite the higher NMR sensitivity of these nuclei), possibly due to a lower electron density at the nucleus for these heavier atoms.

From the analysis of the room temperature data in terms of a Korringa relation, we think it to be most likely that the line splitting at 100 K finds its origin in a modulated charge density at the Yttrium site, which would reflect charge modulation in the nearby copper-oxygen planes. This modulation is possibly associated with the development of a charge density wave due to 1D or 2D-nesting of the Fermi surface [3]. From the present experiment we cannot discriminate between just a doubling of the unit cell or an incommensurate modulation, since both give rise to a split spectrum.

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