Polarized Neutron Scattering Study of Lightly Doped Superconducting YBCO6.33 (T_c = 8.5 K)

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High temperature superconductors (HTSC) have a complex phase diagram. Hole doping drastically changes the magnetic properties of the antiferromagnetic (AF) insulating parent material eventually destroying long-range order. Superconductivity (SC) is observed for doping larger than a critical value (p_c) on the copper oxide planes. Understanding the properties of materials with doping levels close to the boundary of superconducting and long range AF ordered regions of the phase diagram may hold the key to unravelling the mechanism behind HTSC. For $La_{2-x}Sr_xCuO_4$ (LSCO) family, SC emerges from a non-metallic glassy phase whereas the precursor phase for $YBa_2Cu_3O_{6+x}$ (YBCO6+x) remains controversial. To investigate whether SC and long-range AF phases coexist in the YBCO6+x, we have studied a very underdoped crystal of YBCO6.33 with a superconducting transition temperature T_c of only 8.5 K (less than 1/10 of the optimally doped T_c = 94 K) and a hole density of only p ~ 0.055.

Our unpolarized neutron scattering study of the spin spectrum at low-energies in YBCO6.33 indicated [1] that there is no coexistence of superconductivity with long range ordered antiferromagnetism. Instead, we found that at low temperatures an elastic peak at the AF position ***Q*** = (0.5 0.5 L) with L = integer starts to grow gradually on cooling with no indication of a transition to a new phase. Although this peak remains resolution limited in energy, it has a finite width in *Q*-space both for spin correlations within the plane (~ 100 Å) and between planes (~ 25 Å). These short-range correlations indicate the coexistence of a glassy phase within the SC phase. In addition, we found that the spectrum of excitations out of this phase is in the form of a damped Lorentzian with a ~ 3 meV relaxation rate. This study showed that a second-order transition to long range Néel order either lies below the critical concentration for SC or that the transition is first order.

To separate magnetic from nuclear scattering as well as to investigate whether the central mode and its excitations exhibit a preferred spin orientation, we polarized the neutron beam at the C5 spectrometer. Flat Heuser-111 crystals were used both as monochromator and analyzer with a fixed final energy of E_f = 3.52 THz and collimations were set to (0.8°, 0.85°, 2.4°) after the monochromator. No Soller collimation was used before monochromator resulting a 0.6° distance collimation (this is indicated as "none" in the collimations listed on the figures). A Mezei flipper coil was placed on the incident side and one graphite filter was used on the scattered side to suppress higher order neutrons. The Mezei flipper allowed spin-flip (SF) and non-spin-flip (NSF) cross sections to be measured. To control the direction of the neutron spin at the sample position two pairs of coils were used to apply a weak magnetic field (of ~ 3-5 G) either perpendicular to ***Q*** (vertical, VF) or parallel (horizontal, HF) to it (see Figure 1). Flipping ratios of ~ 15:1 and ~ 12:1 were measured for the vertical field and horizontal field configurations, respectively, using several Bragg reflections including (114) as well as using the straight through beam with the sample angle at the (114) position. For inelastic scans, the optimal flipping current at a given energy transfer was set automatically by the control program using an empirical relation between the flipping current and the initial energy (E_i). This relation was determined by measuring the optimal current at several initial energies using the straight through beam and was confirmed by measuring the flipping ratio at several Bragg reflections with final energies of E_f = 3.52 and 7.37 THz.

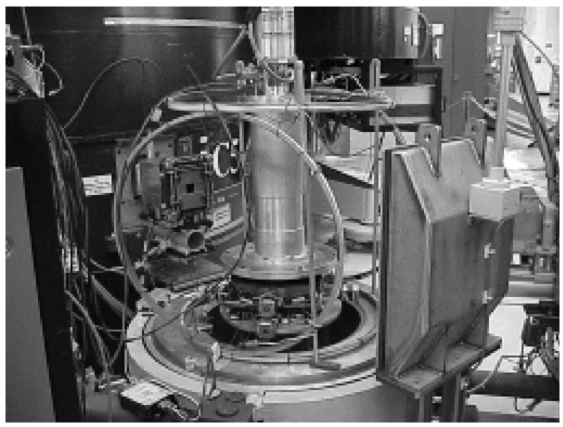

Fig. 1 Two pairs of coils were used to control the direction of neutron spin at the sample position. The sample is mounted in the closed-cycle refrigerator (centre).

For each field configuration at the sample position, the sample was first warmed to 50 K and then field-cooled to low temperatures to prevent any possible depolarization from trapped flux in the Meissner state. For the horizontal field configuration, it was confirmed that during scans the field direction with respect to ***Q*** did not change more than a few degrees, hence the effects of depolarization on the neutron beam was minimal. For the vertical field configuration, the field orientation with respect to the sample was always perpendicular to the scattering plane, i.e. perpendicular to ***Q***.

Since neither the polarizer nor analyzer are perfect, there is always a small number of neutrons with the wrong spin state that pass through and are counted at the detector. To correct for this and obtain the true SF scattering from the measured SF and NSF count rates, we used the following relation [2]

$$SF = C_{SF}\,\frac{F}{F-1} - C_{NSF}\,\frac{1}{F-1}$$

where F is the flipping ratio and C_{SF} and C_{NSF} are the measured SF and NSF count rates, respectively. Similarly the true NSF scattering was determined by the following correction

$$NSF = C_{NSF}\,\frac{F}{F-1} - C_{SF}\,\frac{1}{F-1}$$

The spin correlations, $S^{\alpha\alpha}(\boldsymbol{Q}, \omega)$, in the 2D CuO_2 planes along the [1 -1 0] α direction can be directly determined free of nuclear incoherent or phonon scattering (see Figure 2) by calculating the difference in the SF intensities of the HF and VF configurations (HF-VF) with the sample aligned in the (HHL) plane. In addition, a comparison of the observed SF intensity for HF vs. VF provides some information on the anisotropy of the magnetic scattering along the *ab*-plane vs. *c*-axis direction. For example, if the observed SF scattering for HF is twice as that for VF, the magnetic scattering along different directions is the same showing that the spin orientation is isotropic.

	$H_o \parallel Q$		$H_o \perp Q$	
	SF	NSF	SF	NSF
Nuclear coherent	0	1	0	1
Nuclear isotope incoherent	0	1	0	1
Nuclear spin incoherent	2/3	1/3	2/3	1/3
Magnetic	s_x+s_y	0	s_y	s_x

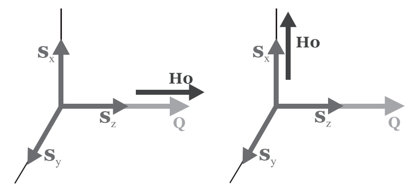

Fig. 2 Two configurations of the neutron spin at the sample position are shown. For each orientation, the contributions from nuclear and magnetic scattering are listed for both the spin-flip (SF) and non-spin-flip (NSF) components. The spin scattering cross-section $S^{\alpha\alpha}$ is denoted $\mathbf{s}_\alpha$.

The polarized neutron scattering results confirm that both elastic and inelastic scattering observed previously with non-polarized neutrons are entirely magnetic in origin. Thus the methods we used in background subtraction for both scattering components correctly gave the magnetic component. The scattering is short ranged and is peaked at AF position (0.5 0.5 L) with L = integer. A comparison of the polarized with non-polarized data is provided in Figure 3 where the magnetic scattering obtained at low temperature along the (0.5 0.5 L) direction is shown.

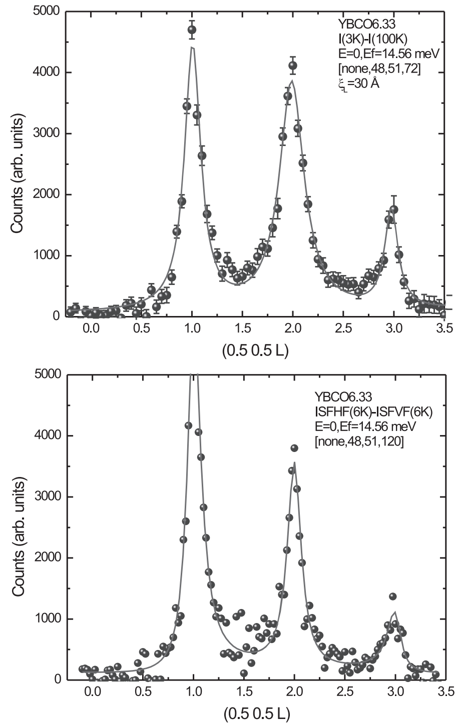

Fig. 3 Elastic magnetic scattering along the (0.5 0.5 L) obtained from the non-polarized study (top, low temperature minus high temperature background) compared to the polarized data (bottom, low temperature SF vertical field data is subtracted from the horizontal data).

Typical H- and L- elastic SF scans are shown in Figure 4 for HF and VF configurations. It shows that the SF scattering with the horizontal field configuration is always twice that measured in the vertical field configuration. This is seen for scans both along the H- and L-directions and indicates that the spin coupling is unpolarized or paramagnetic in nature unlike the undoped parent compound where a strong anisotropy orients the spins preferentially in the *ab*-plane rather than along the *c*-axis.

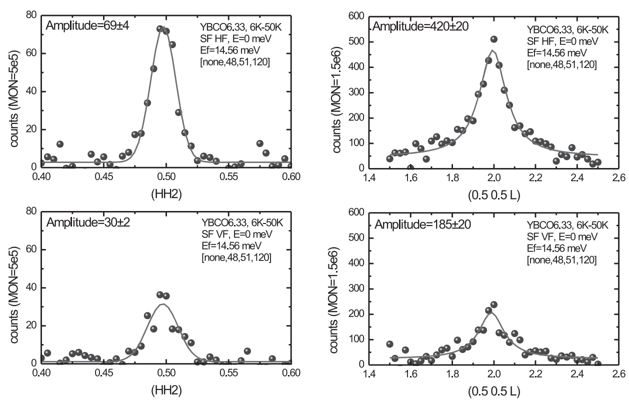

Fig. 4 SF scattering observed along the (HH2) for the HF (top left) and VF (bottom left) configurations. Similar scans are shown on the along the [0.5 0.5 L] direction (right panels).

Our polarized data proves that the unpolarized response previously found to consist of two energy scales, a slow central peak response and faster spins relaxing at a rate of ~ 3 meV, does in fact arise from the magnetic spins. The inelastic spectrum obtained from the difference between

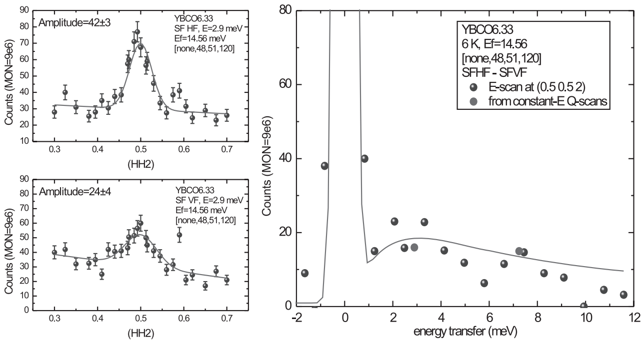

Fig. 5 *Polarized spin-flip inelastic neutron scattering data. Inelastic scans along [HH2] direction (left) show that the spin directions are isotropic since the HF intensity is twice that for VF. (right) The magnetic spectrum along [1,-1,0] measured by subtracting the VF from the HF data. The spectrum is fitted to a central mode and a modified Lorentzian (right line in the right panel).*

the horizontal spin-flip channel and the vertical field spin-flip channel as a function of energy transfer is shown in Figure 5. For inelastic scattering, we also find that the horizontal field SF scattering is always twice that measured in the vertical field configuration again indicating that the spin fluctuations are unpolarized or paramagnetic in nature.

The polarized study shows that the spin response is isotropic unlike the AF undoped parent compound with a strong in-plane anisotropy. It also confirms that the spin correlations coexist with superconductivity and remain short-ranged within CuO_2 planes and perpendicular to them, even for this very underdoped sample close to the edge of the superconducting phase. We conclude that the spins at this low doping are organized into a glassy state with unbroken orientational spin symmetry that coexists with superconductivity below T_c. Hence even lower doping than in YBCO6.33 is required for the long range AF phase to emerge.

References

[1] Z. Yamani et al., Physica C 460–462 (2007) 430.
[2] A.R. Wildes, Rev. Sci. Instrum. 70 (1999) 4241.