TWO-DIMENSIONAL GEOMETRY OF SPIN EXCITATIONS IN THE HIGH-TRANSITION-TEMPERATURE SUPERCONDUCTOR $YBa_2Cu_3O_{6.85}$

V. Hinkov[1], S. Pailhès[2], P. Bourges[2], Y. Sidis[2], A. Ivanov[3], A. Kulakov[1], C. T. Lin[1], D. P. Chen[1], C. Bernhard[1] and B. Keimer[1]

[1] Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany
[2] Laboratoire Léon Brillouin, CEA-CNRS, CEA-Saclay, 91191 Gif-sur-Yvette, France
[3] Institut Laue-Langevin, 156X, 38042 Grenoble cedex 9, France

The fundamental building block of the copper oxide superconductors is a Cu_4O_4 square plaquette. In most of these materials, the plaquettes are slightly distorted and form a rectangular lattice. An influential theory of high temperature superconductivity predicts that this two-dimensional lattice is intrinsically unstable towards a “striped” state with *one-dimensional* spin and charge order [1,2]. Static stripe order has indeed been reported in specific layered copper oxides in which superconductivity is suppressed, but the theory also predicts phases in which robust superconductivity coexists microscopically with liquid-crystal-like stripe order. The liquid-crystal order parameter is expected to align itself preferentially along one of the axes of the rectangular lattice, generating a quasi-one-dimensional pattern in scattering experiments [3].
Testing this prediction requires “untwinned” specimens in which the orientation of the rectangular lattice is maintained throughout the entire volume. However, almost all neutron experiments thus far reported have been carried out on fully ‘twinned’ crystals with equal proportions of micrometre-scale twin domains in which the rectangular Cu_4O_4 plaquettes are rotated by 90° with respect to one another. Because the scattering pattern from such crystals consists of equal contributions from both twin domains, even perfectly one-dimensional spin fluctuations generate a fourfold symmetric pattern, so that they cannot be discriminated from microscopically two-dimensional fluctuations. The results of previous neutron scattering experiments on partially detwinned $YBa_2Cu_3O_{6+x}$ crystals have been interpreted as evidence of a one-dimensional character of the magnetic fluctuations [4]. However, owing to significant contributions from the minority domain, the full geometry of the excitation spectrum has remained unclear.
Using neutron scattering from a mosaic of fully untwinned, nearly optimally doped $YBa_2Cu_3O_{6.85}$ crystals [4], we have resolved this issue. Scans through the (200) and (020) Bragg reflections of the $YBa_2Cu_3O_{6.85}$ array reveal a bulk population ratio between majority and minority twin domains of about 95:5 (Fig. 1b) [5].This is one order of magnitude larger than in previous experiments[4]. The contribution of the minority domain to the magnetic scattering pattern is thus negligible in our experiments.

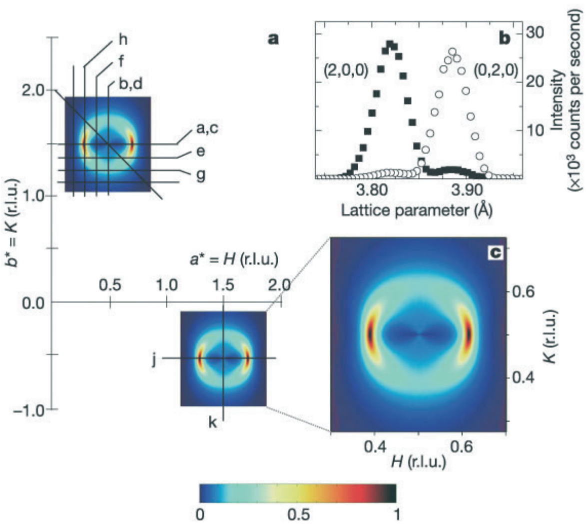

Figure 1. Layout of the reciprocal lattice and magnetic spectral weight of YBa2Cu3O6.85. a) In-plane projection of the $YBa_2Cu_3O_{6.85}$ reciprocal lattice indicating the trajectories of the constant-energy scans shown in Fig. 2.. b) Longitudinal elastic scans through the (2, 0, 0) and (0, 2, 0) crystallographic Bragg reflections, demonstrating a twin domain population ratio of (95:5). C) Intrinsic magnetic spectral weight at 35 meV (see text).

Figure 2 shows magnetic neutron scattering data from this crystal array. The overall features of the neutron cross-section are in good agreement with prior work on twinned crystals. The observed magnetic excitations are incommensurate (Fig 2) around the in-plane wave vector $\mathbf{Q}_{AF}$ =(0.5, 1.5). The incommensurate excitation branches disperse towards $\mathbf{Q}_{AF}$ with increasing excitation energy (Fig. 2), and they merge at 41 meV, giving rise to the ‘resonance peak’.
The new aspect of this work is the determination of the in-plane geometry of the spin excitations. Figure 2c–j shows representative scans from a

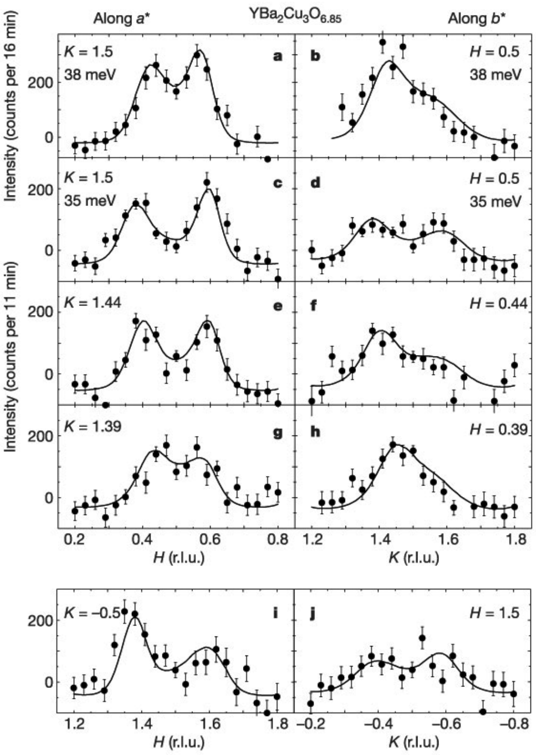

Figure 2. Constant-energy scans along the trajectories indicated in Fig. 1a. The excitation energies are $\hbar\omega =$ 38 meV (a, b) and 35 meV (c–j). The wave vector Q = (H, K,1.7) is given in reciprocal lattice units, r.l.u.. We show subtractions of the intensities at T = 10 K (<<Tc) and T = 100 K (>Tc). The data in panels c, d and i, j were taken in two different Brillouin zones with exchanged resolution conditions. The observed anisotropy between a* and b* is thus not due to resolution effects.

comprehensive map of the spin fluctuation spectral weight at $\hbar\omega$=35 meV. More limited data sets were also taken at $\hbar\omega$= 33 and 37 (not shown), and 38 meV (Fig. 2a,b). The most important observation is that well-defined incommensurate peaks are present in scans along both a* and b* (Fig. 2a-d). This demonstrates the intrinsic two-dimensional nature of the spin excitations. To extract the magnetic spectral weight from the experimentally determined scattering profiles, we have numerically convoluted an anisotropic damped harmonic oscillator cross-section with the spectrometer resolution function. The computed profiles, shown as solid lines in Fig. 2, provide excellent descriptions of the experimental data. We find that the locus of maximum spin fluctuation spectral weight approximately forms a circle in momentum space, in agreement with its two-dimensional geometry. However, the damping and amplitude along the circle are modulated in a one-dimensional fashion. The intrinsic magnetic spectral weight at 35meV extracted from this analysis is depicted in Fig. 1c. The strength of this modulation also depends strongly on the excitation energy.

Which models can describe the observed one-dimensional amplitude and width anisotropy? i) Theories based on a one-dimensional, rigid array of stripes predict a 100% intensity anisotropy and cannot account for the two-dimensional scattering pattern. The map of the magnetic intensity at 35meV does, however, bear a resemblance to the scattering pattern generated by a nematic liquid crystal close to a nematic-to-smectic critical point [3]. In this scenario, the structural anisotropy between the a and b axes may act as an aligning field for the nematic director.

ii) Prior Fermi-liquid-based theoretical scenarios for the spin dynamics of $YBa_2Cu_3O_{6+x}$ had only considered independent CuO_2 layers, ignoring a possible influence of the b-axis-oriented CuO chains [6]. Their impact (via an orthorhombic anisotropy) on the spin dynamics has to be assessed in quantitative calculations. Other factors, such as proximity to a 'Pomeranchuk' instability of the Fermi surface [7], may also contribute to the anisotropy of the spin dynamics.

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