Antiferromagnetic domains in $YBa_2Cu_3O_{6.0}$ detected by neutron Larmor diffraction

B. Náfrádi[1], T. Keller[1], A. Erb[2], B. Keimer[1]

[1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
[2]Walther-Meißner-Institut für Tieftemperaturforschung, Garching, Germany

High resolution Neutron Larmor diffraction measurements at TRISP helped to resolve a long standing problem related to an anomalous magneto-resistance observed in $YBa_2Cu_3O_{6.0}$ [1]. This compound is a two-dimensional antiferromagnet and becomes superconducting at higher oxygen doping levels. In this work we observed a small broadening of the Bragg peaks arising from an orthorhombic distortion of the crystal lattice in the order of $(b-a)/b = 2.6 \cdot 10^{-6}$. This distortion appears reversibly in the antiferromagnetic state and results from magnetostriction induced by antiferromagnetic domains. From the anisotropic broadening of the Bragg peaks we found that in the a-b plane the domains are larger than 10^4 unit cells.

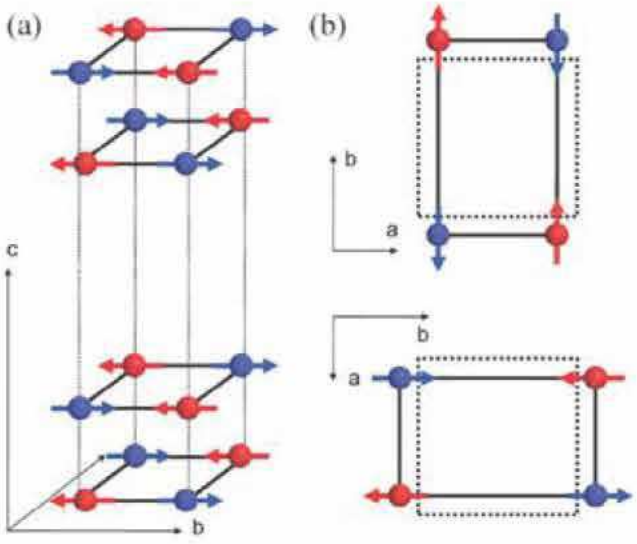

Figure 1 (a) Schematic view of the average tetragonal antiferromagnetic structure of $YBa_2Cu_3O_6$ below the Néel temperature $T_N = 420$ K. For clarity only the magnetic Cu^{2+} ions are shown. (b) The two types of orthogonal domains resolved at TRISP. Dashed rectangles represent the tetragonal paramagnetic unit cell. The solid rectangle represents the orthorhombic antiferromagnetic cell. The direction of both the orthorhombic distortion and the easy magnetization rotates 90° between domains.

Antiferromagnetic domains

The high-Tc cuprate superconductors are based on insulating antiferromagnetic parent compounds, such as the $YBa_2Cu_3O_{6.0}$ studied in this work. Superconductors are obtained by doping the parent compounds with charge carriers. A detailed description of the magnetism of the parent compounds is assumed to be a key for understanding the superconductivity [1-4].

An open question is related to the observation of an anomalous magnetoresistance within the CuO planes. One of the scenarios discussed as an explanation for this effect assumes an orthorhombic distortion of the crystal lattice resulting from orthogonal antiferromagnetic domains. The formation of antiferromagnetic domain walls costs energy and should, therefore, be forbidden. However, if strong magneto-elastic coupling is present, the long range magneto-elastic forces lead to an energetically favorable lattice distortion and spontaneous domain formation can occur [4] (fig. 1).

Precise diffraction

Using high resolution neuron Larmor diffraction (LD), we were able to confirm the existence of a small orthorhombic distortion of $(b-a)/b = 2.6 \cdot 10^{-6}$ and twinning below the Neel temperature [8]. The sample consisted of small co-aligned crystals with a total crystal mass of 10mg. Larmor diffraction [6,7] is a diffraction technique implemented at the TRISP spectrometer at the MLZ (fig. 2), a spin-echo technique providing a relative resolution for the lattice spacing or the spread of the lattice spacing in the order of 10^{-6}, that is, about 1–2 orders of magnitude better than the resolution obtained with conventional neutron or X-ray diffraction techniques. In

addition to making it possible to detect a small splitting of Bragg peaks, Larmor diffraction is an unrivalled method for measuring thermal expansion under extreme conditions not accessible by classical dilatometry, including high pressure and low temperature. We found that the orthorhombic distortion and domain structure is caused by magnetostriction, and the structural domains presented in this work are identical with magnetic domains reported earlier. [2,4] From the anisotropic broadening of the Bragg peaks, we found that, in the a-b plane, the domains are larger than 10^4 unit cells.

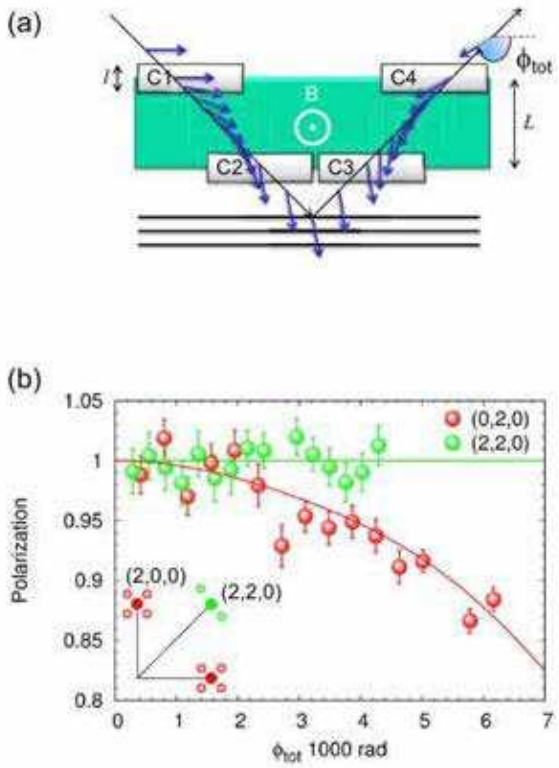

Figure 3 (a) Principle of the Larmor diffraction technique. The radio-frequency spin flip coils C1 to C4 generate an effective (virtual) static magnetic field B, leading to Larmor precession of the neutron spins. The total precession phase only depends on the lattice spacing and is independent of beam collimation and monochromaticity. (b) Normalized neutron beam polarization as a function of the total Larmor precession phase measured at T = 300 K (T_N = 420 K) for both (2,2,0) and (2,0,0) nuclear Bragg peaks. The fast decay of the (0,2,0) polarization results from the orthorhombic twinning shown in the inset. Full circles mark the reciprocal lattice points of the paramagnetic tetragonal phase.

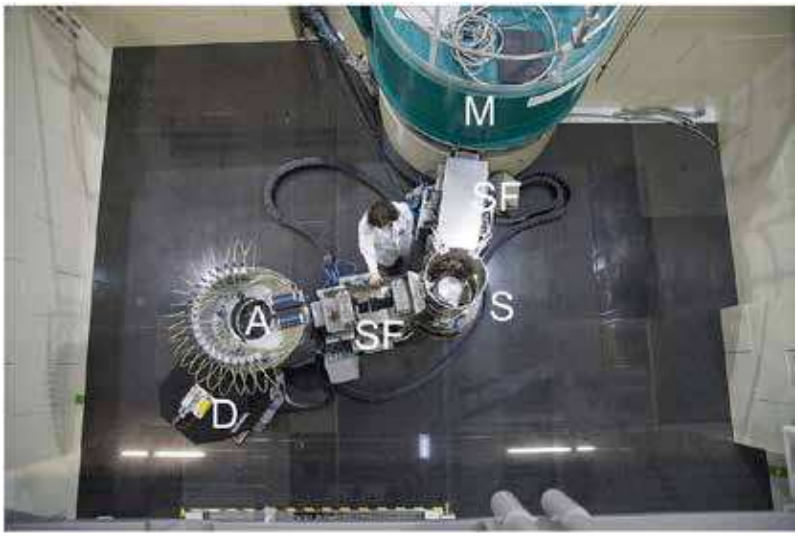

Figure 2: The TRISP (TRIple axis SPin echo) spectrometer at the MLZ is optimized for high resolution spectroscopy of elementary excitations by means of resonance neutron spin echo. It incorporates the Larmor diffraction technique. The lattice spacing and the spread of the lattice spacing arising, for example, from defects, internal strain or small splitting of Bragg peaks is measured with a relative resolution in the order of 10^{-6}, i.e. 1–2 orders of magnitude better than other diffraction techniques. The method works both for single-crystals and powders. (M: monochromator; SF: radio frequency spin flippers housed in a μ-metal shield; S: sample; A: analyzer; D: detector)..

Acknowledgements

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