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Vortex lattice accommodation on twin boundaries in $YBa_2Cu_3O_7$ studied by neutron diffraction

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Abstract. An extensive study of small angle neutron scattering was performed in twinned $YBa_2Cu_3O_7$ crystals in its superconducting state as a function of the angle θ_B between the c-axis of the crystal and the magnetic field. The half of the twin boundaries are oriented in the horizontal plane, which also contains the neutron beam and the magnetic field. Two different diffraction patterns are studied as a function of θ_B at 5 K and $B = 0.5$ T, one along the c-axis of the crystal, the other one along the applied field. These variations are interpreted in the model of accommodation of the vortices on the twin planes by zigzagging from these planes to the ab-planes of the crystal, in order to minimize their energy.

PACS. 74.72.Bk Y-based cuprates – 74.60.Ge Flux pinning, flux creep, and flux-line lattice dynamics

1 Introduction

The behavior of flux lines in $YBa_2Cu_3O_7$ is of great importance to understand the flux pinning and hence the critical current for most of practical applications. In this compound, the role of the pinning is still controversial: most of the papers claims that the pinning is due to microstructural defects such an inclusions, microcracks [1–4], but others an in favor of nanostructural defects (oxygen vacancies) [5]. Twin boundaries are also important in transport properties [6], but their exact effect is still unknown. Recent scanning tunneling microscopy studies did show that the role of the twin boundaries is very important in the orientation of the vortex lattice [7]. Among all the experimental techniques, neutron diffraction probes directly the bulk structure of the vortex lattice. Different observations have conclude by this technique that the twin boundaries play an important role, since a square pattern is often observed when the field is applied along the c-axis [8–10]. Other authors have interpreted these data by suggesting that the symmetry of the superconducting order parameter is important in stabilizing this structure [11, 12], but this is still controversial [12]. When the field is tilted away from the c-axis, the structure becomes quite complicated [8–10].

In an energetic analysis, Blatter *et al.* [13] have proposed that the vortices can meander to follow the twin boundaries in the ab-plane. To interpret some transport data in presence of columnar defects [14], it is sometimes also suggested that an accommodation of the vortices on the defects which should zigzag from the defects to a direction close to the ab-plane or a decomposition of the vortex lattice can occur. This would minimize the energy [15].

In this article, we try to use the model of the accommodation of the vortices to interpret small angle neutron scattering (SANS) experiments on two twinned crystals of different twin boundary density. We study in particular the angular dependence of the vortex lattice as function of the applied field direction.

2 Experimental details

The first sample, named I, has been prepared by melt textured growth process [16]. From a previous study [17], it was shown that for the critical current point of view an optimum composition is obtained for $YBa_2Cu_3O_7$ + 20% $YBaCuO_5$ + 21% CeO_2 + 0.5% PtO_2. From scanning electron microscopy, the polished surface exhibits an homogeneous distribution of Y_2BaCuO_5 inclusions of about few microns. Small cubic inclusions of $BaCeO_3$ are also observed. High resolution transmission electron diffraction allows us to measure the average distance between twin boundaries (500 Å). This quite small value, compared to literature, can be related to the high critical currents observed in this sample (7×10^4 Å/cm^2 at 77 K in transport measurements and up to 10^4 Å/cm^2 with 6 T applied along the c-axis). A small part ($1 \times 1 \times 2$ cm^3) was extracted from the bar for the neutron study. A second

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sample, named II, was prepared in a different way [18] and presents an average distance between twin boundaries of about 1200 Å. The sample was prepared from a mixture of commercial powders Y123, Y211 (43 wt% in excess) and PtO_2 (0.5 wt% in excess) pressed at 80 MPa under an uniaxial load into a disc pellet of 25 mm diameter. The pellet was textured in a box furnace using a top seed melt texturing method with a Sm123 seed. A large oriented single domain crystal was obtained into which a $14 \times 14 \times 9$ mm^3 parallelepiped was cut, the square section being parallel to the *ab*-plane. Both samples were annealed at 480 °C under pure oxygen for a week to reach a critical temperature of about 92.5 K.

SANS experiments were performed on the spectrometer PAXY at LLB (Saclay, France). The multidetector (128×128 cells of 05×05 cm^2) is located at 7 m from the sample. The sample was placed in a variable temperature cryostat fixed on the goniometer and the rotation table of the spectrometer. The *c*-axis of the samples were oriented *in situ* by the observation of the Bragg peak 001 using a 4.39 Å and a scattering angle of the detector of about 22°. For the vortex scattering study, we have used a neutron wavelength of 10 Å with a mechanical selector $\delta\lambda/\lambda$ of about 10%. At room temperature, the samples exhibit the classical SANS of twinned crystals [8]. It has a typical cigar shape, with the large dimension along *c*-axis perpendicular to the neutron beam. With the neutron beam parallel to *c*-, the pattern is mainly due to twin boundaries. The cross shaped of the pattern allows us to orientate the twin planes (110) and (1,−1,0), noted t and t' in the following. The t'-axis was put in the vertical direction. with this experimental setup, another rotation table was used to vary the magnetic field direction in the horizontal plane from *c*- to *t*-axis. With this experimental setup, it is possible to rotate the field in the horizontal plane from *c*- to *t*-axis. θ_B is the angle between B and c in the following. The angular resolution of the incident neutron beam was chosen large on purpose (0.15°), in order to observe the vortex lattice Bragg peaks on the detector without any rotation ω of the sample. Such a procedure is valid for the large Bragg plane spacing of the vortex lattice in the SANS experiments.

In the superconducting state, the diffraction pattern exhibits an additional signal which can be clearly evidenced by the subtraction of a 100 K spectrum, taken as a background. A the magnetic diffraction patterns were recorded at 5 K.

3 Experimental results

First, we study the vortex lines which lie in the direction of the magnetic field. Figure 1 presents the typical diffraction patterns observed at 5 K and $B = 0.5$ T at different angles θ_B when the incident neutron beam is parallel to the applied field. There are the typical "hexagonal" patterns already observed in $YBa_2Cu_3O_7$ [9] when the magnetic field is tilted away enough from the *c*-axis. The six spots are located on an ellipse. The ratio R of the axis lengths

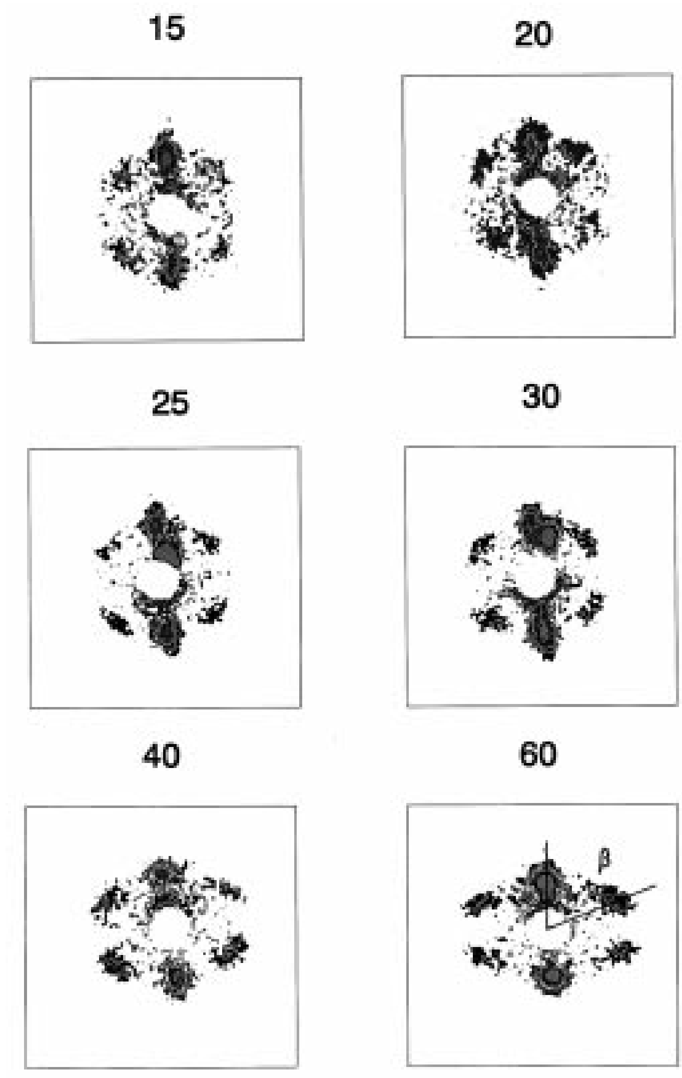

Fig. 1. The diffraction patterns obtained with the incident neutron beam aligned to B at different angles between B and *c*-axis (0.5 T, 5 K, sample I).

is given by (the anisotropy γ of the material is about 5 here) [19]:

$$R^2 = (\cos^2\theta_B + \sin^2\theta_B/\gamma^2). \quad (1)$$

Compared to the typical diffraction pattern of a triangular lattice, important differences are observed: the two vertical spots in the direction of the twin planes are more intense than the four other ones. This can not be due to a problem in the Bragg conditions since the angles are very similar. Moreover, the intensity of these four spots decreases as the angle θ_B decreases: it is not measurable when θ_B tends to zero. The angular position of these peaks is also different from they should be in a triangular lattice distorted by the anisotropy. The q value of these peaks are

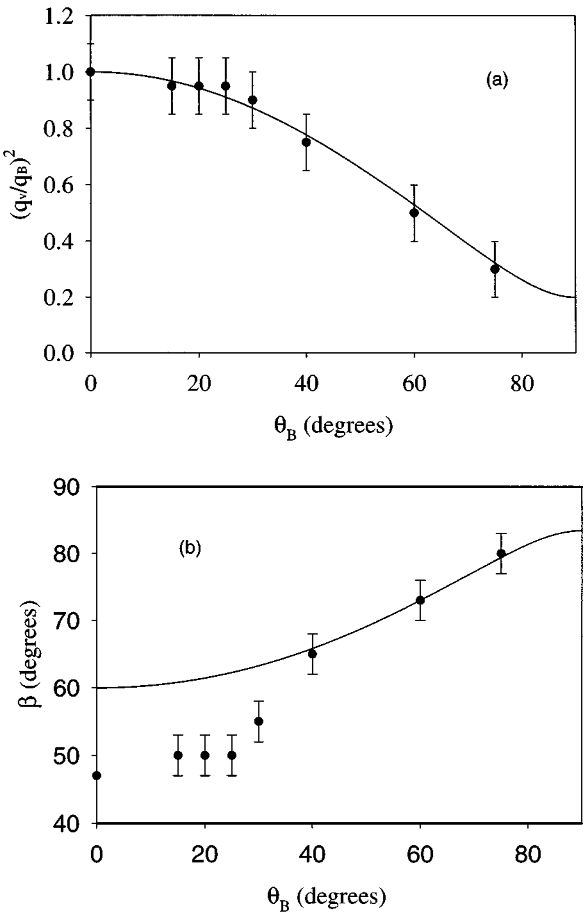

Fig. 2. (a) The angular dependence of the position of the vertical spots of Figure 1. The solid line corresponds to R given by equation (1) in the text. (b) The angular dependence of the angle β as defined in Figure 1. The solid line is given by equation (4) in the text.

given in this case by [19]:

$$q_V = R^{1/2} q_B \cos\beta$$
$$q_H = R^{-1/2} q_B \sin\beta \qquad (2)$$

where q_V and q_H are the vertical and horizontal components of the wave vector of the peak. The value of q_B indeed corresponds to the calculated value

$$q_B = 1.07 \quad 2\pi \left(\frac{B}{\Phi_0}\right)^{1/2} \qquad (3)$$

indicating that it corresponds to the applied field (Fig. 2a). The corresponding angle β (shown in Fig. 1) between the spots and the vertical axis is reported in Figure 2b as a function of θ_B. On this figure, we have also reported the calculated value of β in a triangular lattice of an anisotropic superconductor:

$$\mathrm{tg}\beta = \mathrm{tg}(60°)/R. \qquad (4)$$

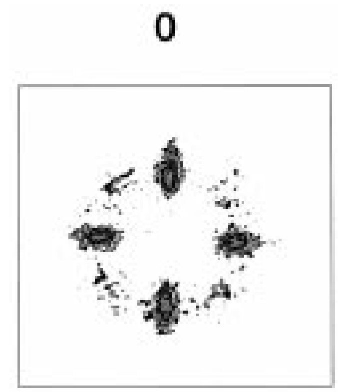

Fig. 3. The diffraction pattern when B, c and the neutron beam are aligned (0.5 T, 5 K, sample II).

A distortion of the observed lattice is clearly obtained for small θ_B values. The extrapolated value at $\theta_B = 0$ was already reported at 47° [12] in agreement with the present data. Such a distortion from the hexagonal symmetry to a square lattice with the angle θ_B was already observed in other systems such as YNi_2B_2C [20] but the interpretation is not clear.

When θ_B is exactly zero (within 1°) two horizontal peaks with the same q vector and the same intensity as the two vertical peaks appear (Fig. 3). This diffraction pattern was also previously observed by other authors [8–10]. In this geometry, the integrated intensity of the spots was estimated taking into account the angular dispersion of the beam to be equal to the value it should be [21]:

$$I = I_0\, 4.5 \left(\frac{1.91}{2}\right)^2 V \lambda_n^2 \left(\frac{q}{2\pi}\right)^3 \left(1 + \lambda^2 q^2\right)^{-2} \qquad (5)$$

where $\lambda = 1670$ Å is the London length, V is the sample volume, $\lambda_n = 10$ Å the neutron wave length, I_0 the incident neutron flux and q is the Bragg vector: we have checked by this measurement that it is not a small part of the sample which is responsible for the magnetic signal observed in this geometry.

Following the work of Forgan *et al.* [8], we have also investigated the magnetic diffraction pattern observed in the c-axis direction, when the field is trapped at an angle θ_B to the c-axis. In this geometry, the presence of the coils of the magnet prevents the direct study of the scattering for angles θ_B between 20° and 60°. Thus, we have performed the experiment by field cooling to 5 K and then removing the field. The pinning at 5 K is strong enough to keep the field in the sample and to observe the vortex lattice. Figure 4 presents the diffraction pattern of sample II along the c-axis direction for different values of θ_B. It can be seen on this figure that the vertical peaks already observed in the direction of the magnetic field are also visible in this direction. This is normal since the only difference is a rotation around the vertical axis of the sample together with the vortex lattice. Two additional peaks at low q values can be also observed on the horizontal axis, revealing

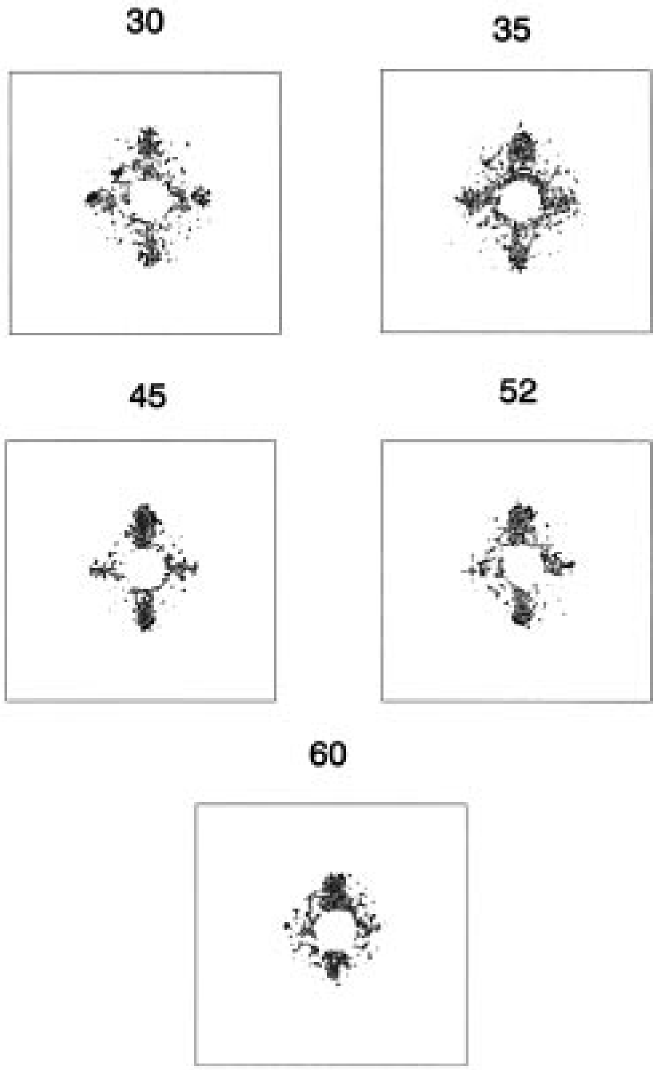

Fig. 4. The diffraction patterns obtained in the c-direction for different values of θ_B (0.5 T, 5 K, sample II).

an additional periodicity in this direction and the persistence of part of the vortices in this direction. The ratio between the horizontal periodicity and the vertical one is shown in Figure 5. This ratio is fitted by $\cos\theta_B$ on the same figure, with a very good agreement. When the angle θ_B becomes larger than 60°, the spots are not visible due to the presence of the beam stop.

We have performed the same measurements on sample I which presents a larger density of twin boundaries. Though at 0.5 T, the vortex-vortex distance (700 Å) is smaller than the twin periodicity (1200 Å), this is not the case in sample II where the average twin periodicity is 500 Å. Nevertheless, the positions of the peaks observed on the diffraction patterns are very similar in the two samples.

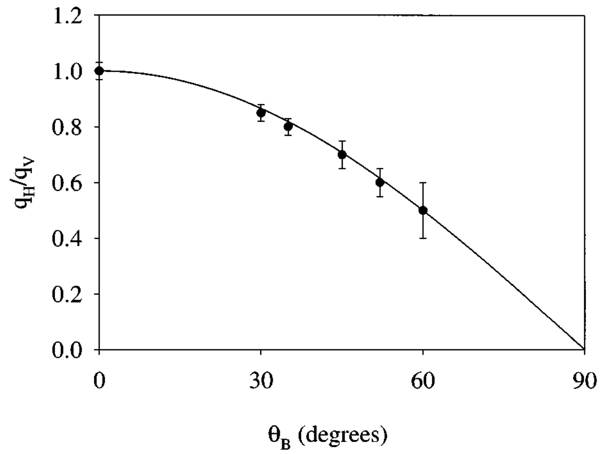

Fig. 5. The angular dependence of the ratio of the horizontal and vertical periodicities defined in Figure 4. The solid line is $\cos(\theta_B)$.

4 Discussion

Different interpretations have been proposed to account for these observations in the past. Forgan *et al.* [8] first suggested that twin boundaries can be at the origin of these effects without any precise model. Then, other authors [11,22] argued that the symmetry of the order parameter of the superconducting state can be at the origin of this phenomenon. We propose a precise model of vortex meandering which provides some diffracted intensity in a plane which is not perpendicular to the magnetic field. This can be understood only if the vortices are not straight lines.

Let us first remind that the magnetic field in the sample roughly follows the applied field for field cooled measurements well above H_{c1}. This is here the case. In the accommodation of the vortices on the twin planes, as proposed by Blatter *et al.* [13], Ettouhami *et al.* [15] and by Hardy *et al.* [14], the vortex meanders in a zigzag from the twin planes to an other direction close to the *ab*-plane. In their paper, Ettouhami *et al.* have estimated that the minimization of the energy should be in favor of the decomposition of the vortex lattice into two sublattices: one along the c-axis, the other one along the *ab*-plane. In this case, when the diffraction is measured along the c-axis, q_V should be equal to q_H, whatever the θ_B angle is. In our samples, the diffraction in the c-direction gives an anisotropic pattern with an anisotropy ratio of $\cos\theta_B$ (Figs. 4 and 5). On the contrary, the accommodation model, though it should be a little less energetically favorable, can account for this ratio, as we will discuss in the next paragraph.

In the accommodation model, it is assumed that all the vortices contribute to both patterns. Then, the corresponding vortex density should be very close to that which corresponds to the applied field. In this model, it is predicted that the **q** vector of the vertical spots should vary in $R^{1/2}$. This is experimentally verified in Figure 5 as it

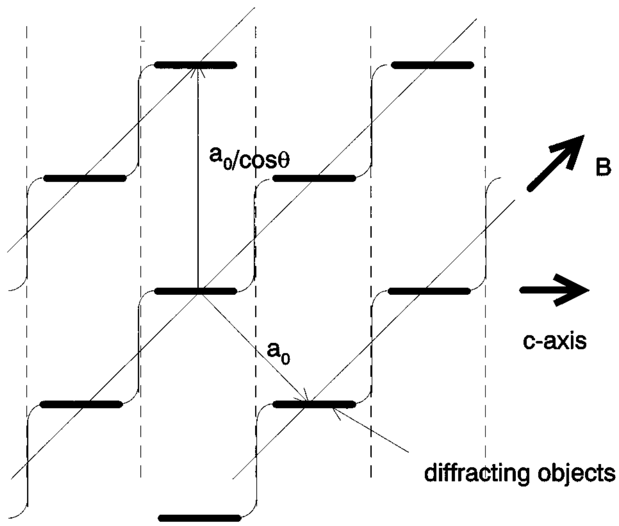

Fig. 6. The schematic drawing of the vortices in the accommodated state (note that in fact, the zigzag is in a plane which does not correspond to the a_0 vector. They are presented here in the same plane for simplicity of the drawing). The two periodicities are shown on the figure (a_0 and $a_0/\cos\theta_B$).

was plotted in Figure 2a for the other sample. The difficulty is to account for the horizontal spots observed when the diffraction is made in the direction of the c-axis (the vertical ones are the same in the B and c directions since the vertical axis is the axis of the rotation). Within this model, the presence of diffracted intensity out of the plane perpendicular to the B direction implies that the vortices are not straight lines. In Figure 6, we have represented a possible vortex structure which presents the classical periodicity a_0 between the average position of the vortices, but also a periodicity in a direction perpendicular to the c-axis. Since the London length is quite anisotropic, only the portions of the vortices parallel to the c-axis contribute significantly to the diffraction. The pattern should then present a diffraction peak when the neutron beam is parallel to this direction as it is experimentally observed. In this model, the Bragg positions along the c-axis are in good agreement with the model as it can be seen in Figure 6: $a_0/\cos\theta_B$. Though this model can account for the diffraction spots, it does not explain by itself why this periodicity appears, *i.e.* what is the interaction which aligns the ab-plane vortex portions. It was proposed in the case of the pinning by the columnar defects that this comes from some attractive interaction between the kinks by entropy effects [23]. In the present case, we imagine that the presence of the twin boundaries induces the meandering of the vortex, and then a similar entropic effect aligns the kinks, giving this new periodicity.

In order to account for the diffraction pattern observed in the B direction, the problem is more complex. The value of the angle β and the intensity of the satellites are very difficult to estimate. If the β value comes from a competition between the vortex pinning and the vortex-vortex interactions, the triangular lattice seems to be more favorable when θ_B is large enough, the square structure is favored by the interaction with the twin boundaries. The existence of an in-plane anisotropy of λ should be also taken into account (comment of Ref. [12]). Finally, it should be possible to make a detailed analysis of the energy of the system as it was done in the case of the columnar defects [13], but the problem is here more complex since the exact interaction between the vortex and the twin plane is not known. The fact that the vortex can be in the twin plane or away from it is still under discussion and this is very important in the evaluation of the pinning energy. Recent scanning tunneling microscopy studies seem to show that they are away from the twin plane which is not superconducting at all [7].

5 Conclusion

Two different magnetic diffraction patterns are observed at 5 K and $B = 0.5$ T, one along the c-axis of the crystal, the other one along the applied field. These two patterns depends on the value of θ_B and were interpreted in the model of the accommodation of the vortices on the twin planes by zigzagging from these planes to the ab-plane of the crystal, in order to minimize its energy, as already discussed by Blatter *et al.* for the twins and by Hardy *et al.* for the pinning by columnar defects. The origin of the θ_B dependence of the angle β is still unknown, though the competition between pinning by twin boundaries and vortex-vortex interaction may be at the origin of this effect.

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Note added in proof

Very recently, a preprint by S.T. Johnson *et al.* (cond-mat archive 9804159) shows that, in a crystal with a much smaller density of twin boundaries, the interaction between the flux lines and the copper oxides chains can also play an important role in the orientation of the lattice in YBaCuO.

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