Inclined-Field Structure, Morphology, and Pinning of the Vortex Lattice in Microtwinned YBa$_2$Cu$_3$O$_7$

B. Kelmer,* F. Doğan, I. A. Aksay, R. W. Erwin, J. W. Lynn, M. Sarikaya

A detailed small-angle neutron scattering study of the vortex lattice in a single crystal of YBa$_2$Cu$_3$O$_7$, was made for a field of 0.5 tesla inclined at angles between 0 and 80 degrees to the crystalline c axis. The vortex lattice is triangular for all angles, and for angles less than or equal to 70 degrees its orientation adjusts itself to maximize the pinning energy to densely and highly regularly spaced twin planes. These observations have important implications for the microscopic flux-pinning mechanism, and hence for the critical current achievable in YBa$_2$Cu$_3$O$_7$. For large angles (about 80 degrees) the vortex lattice consists of independent chains in the orientation predicted by anisotropic London theory.

The nature of the vortex state in the cuprate high-temperature superconductors remains an issue of great theoretical and practical interest. A variety of experimental techniques have been used to investigate the static and dynamic vortex correlations in these materials. In contrast to surface imaging techniques, such as low-field (B ≤ 0.005 T) Bitter decoration (1) or scanning tunneling microscopy (2), neutron scattering is sensitive to the entire length of the vortices in the bulk of the material. Neutron scattering experiments can be performed in a magnetic field range of ~0.05 T up to several teslas, a theoretically interesting regime in which the vortices interact strongly. This is also the relevant field range for prospective magnet applications of the copper oxide superconductors. In fact, the success of our experiments depended critically on the preparation of a large (~2.5-cm diameter, 0.9-cm thickness), high-quality single crystal in a program devoted to device applications of bulk YBa$_2$Cu$_3$O$_7$.

The experiments address two interrelated issues. First, the layered structure of the copper oxides and the concomitant large anisotropy of the electronic properties give rise to complex current and field distributions around individual vortices. The ensuing unusual interactions between vortices can lead to novel vortex structures as the magnetic field is inclined at an angle θ with respect to the c axis (1). By performing neutron experiments for 0° ≤ θ ≤ 80°, we tested these theories in fields up to 0.5 T.

A second issue of great practical significance is the interaction of the vortex lattice with pinning centers that prevent dissipative vortex motion at high temperatures and cause flux trapping at the external field is removed. We carried out extensive electron microscopy studies to identify the microscopic features potentially responsible for flux pinning in our samples. Our neutron measurements indicate that among the possible candidates (inclusions of the nonsuperconducting Y$_2$BaCuO$_3$ phase, stacking faults, and twin planes) only the densely spaced twin planes have a substantial effect on the structure of the vortex lattice. Prior evidence for the importance of twin planes as pinning sites derives mainly from Bitter decoration (2) and transport (4) studies conducted for either θ = 0° or θ = 90°. We show that the vortex lattice orientation locks into the orientation of the twin planes up to a surprisingly large inclination angle θ = 70°. We discuss this observation in terms of microscopic models of the vortex structure. For larger inclination angles, we report the observation of a vortex chain state.

The single-crystal sample was synthesized by a seeding technique in a temperature gradient (5). The characterization of our sample by transmission electron microscopy was carried out by the cutting of several sections perpendicular to the (001) and (110) planes from an identically prepared crystal. A selected-area diffraction pattern with the electron beam in the [001] direction is shown in the inset of Fig. 1. The orthorhombic strain Δa = (b$_O$ - a$_O$)/a$_O$ = 1.8%, Δc = b$_O$, and a$_V$ are the basal-plane lattice parameters in the orthorhombic and tetragonal phases) determined from the splitting of the [110] diffraction peak is identical for several sections of the sample, which proves that oxygen is distributed homogeneously throughout the bulk of the sample. The sample created as the sample is cooled through the tetragonal-orthorhombic transition at 700°C is relieved by the formation of two variants of twin boundaries on the (110) and (110) planes (Fig. 1). As discussed previously (6), the separation D of the twin boundaries is inversely proportional to Δa, so the highly regular twin-plane spacing again indicates a homogeneous distribution of oxygen. By measuring 250 twin domains, we obtained D = 900 ± 30 Å. We determined the width of the twin boundaries to be 15 ± 5 Å from the width of the weak rod of scattering extending in the [110] direction around the [110] diffraction peak of Fig. 1. Because this width is of the order of the in-plane superconducting coherence length, the twin planes may be effective core-pinning sites.

Our coordinate system is defined in Fig. 2. The angles α and φ are determined by the orientation of the crystal by x-ray diffraction outside the cryostat. Once the sample is mounted in the cryostat, the angles θ and φ can be changed by the rotation of either the cryostat inside the magnet or the entire cryostat-magnet assembly, respectively. The crystalline (100) axis was kept in the (x, y) plane and the 110 plane was kept in the (z, y) plane for the diffraction patterns (Fig. 3). The coordinates of the incident beam were fixed at the toroidal angle @ marked 45° and the angle θ varied. The coordinates of the X-ray beam were marked that the incident beam was fixed at the toroidal angle at 45° and the angle α varied.

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*To whom correspondence should be addressed.

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Fig. 1. Electron micrograph showing one family of twin boundaries in our YBa$_2$Cu$_3$O$_7$ crystal. The inset is a selected-area diffraction pattern (20-µm aperture) with the electron beam in the [001] direction, showing the orthorhombic splitting of the diffractions.

Fig. 2. Coordinate system defining our angle conventions. Our experiments were carried out with y fixed at either 0° or 90°, φ fixed at 45°, and θ and φ varied. The coordinates y and z perpendicular to the magnetic field (x axis) are the abcissa and ordinate, respectively, in the diffraction patterns of Fig. 3.
plane to ±3°, so that φ = 45°. We performed the neutron scattering experiments for two different values of χ: 0° ± 1° and 9° ± 1°. It is important to understand the difference between these two configurations: In the first case (χ = 0°), the magnetic field bisects the angle between the two sets of twin planes for any value of θ. In the second case, the c axis is slightly offset from the field direction by χ = 9° at θ = 0°, so that for θ ≠ 0° the angles αc submerged between the magnetic field and the two sets of twin planes are different: αc = sin−1(sin θ ± cos θ sin χ)/√2. This small difference in angle has profound consequences for the structure of the vortex lattice.

The data for χ = 0° and χ = 9° are shown in Fig. 3, A to F, and Fig. 3, G to I, respectively. For θ ≠ χ = 0°, we observe the diffraction pattern with fourfold symmetry reported for large χ angles in Fig. 3A. This result led Yethiraj and co-workers (9) to the conclusion that the vortices form a square lattice, which maximizes the binding energy between vortices and both sets of twin planes, rather than the triangular lattice expected if vortex-vortex interactions dominate. To investigate this point further, we oriented the crystal so that χ = 9° and θ = 5° (Fig. 3C). This small angular offset causes a single-domain triangular lattice to be formed in the entire crystal, as evidenced by the hexagonal diffraction pattern. A fit to the circularly averaged intensity profile gave a peak position (τ) of 0.0092 ± 0.0003 Å−1, somewhat smaller than the value of τ = 2.15μνV/βδ0, = 0.0105 Å−1 calculated from the flux quantization rule for an undistorted triangular lattice (δ0 is the flux quantum). Within experimental error, no such expansion of the average lattice spacing is observed for a larger θ. The slight expansion of the lattice for θ = 0°, together with the significant transverse broadening of four of the reflections, indicates the formation of defects that lead to an accumulation of vortices near twin planes.

Because of the poor longitudinal resolution of our instrument, we can only put a lower bound of ~3 lattice spacings on the translational correlation length. The instrumental resolution in the θ direction is much sharper (~0.2°), and rocking curves in the θ direction revealed an intrinsic width of Δθ = 1° for the Bragg reflections, in agreement with previous measurements (9). The correlation length ξ of the vortex displacement field in the magnetic field direction is given approximately by ξ = (τΔθ)−1 ~ 6000 Å (10). The vortices are therefore significantly deflected from the field direction as they bend and follow the twin plane over some distance to gain advantage of the twin-plane pinning energy (11). In this model, the finite correlation length merely reflects the lack of long-range order in the twin-plane position. The vortex line tension, which opposes this bending, leads to the formation of a single-domain pattern (Fig. 3G): The lowest elastic energy and maximum pinning energy of the vortex lattice are achieved if the orientation of one of the principal axes is given by the set of twin planes subtending the smaller angle α with respect to the magnetic field. The square pattern of Fig. 3A arises simply as a superposition of two orientations that are degenerate for χ = 0°.

The broadening of the θ rocking curves persists up to θ = 45°. However, for θ = 90° the reflections become resolution-limited in all directions. These results are qualitatively consistent with high-temperature transport measurements (6) revealing a drop in the resistivity due to vortex motion when the magnetic field is applied within a “critical angle” with respect to the twin planes (12). It has been suggested (11) that vortex bending becomes energetically unfavorable above this critical angle; our neutron scattering data provide microscopic evidence for such behavior.

We now turn to the position of the Bragg reflections. In the “effective mass” model of an anisotropic superconductor, the reciprocal lattice vectors b1 and b2 of the vortex lattice, in terms of the coordinates y and ξ perpendicular to the magnetic field (Fig. 2), are given by (13)

\[ \mathbf{b}_1 = \frac{\tau}{\epsilon(0)} \left( \begin{array}{c} 0 \\ 0 \\ \cos 60° \end{array} \right) \]

\[ \mathbf{b}_2 = \frac{\tau}{\epsilon(0)} \left( \begin{array}{c} 0 \\ 0 \\ \sin 60° \end{array} \right) \]

for χ = 0°. Here \( \epsilon(0) = \epsilon^* \sin \theta + \cos \theta \), and \( \epsilon^* = m_d/m_c < 1 \) is the effective mass ratio, where \( \epsilon \) is the penetration-depth anisotropy and \( m_d \) and \( m_c \) are the effective masses in the ab plane and along the c axis, respectively. Inspection of the diffraction patterns of Fig. 3, B to E, reveals that although the distortion of the vortex lattice is consistent with Eq. 1, the orientation of the lattice does not follow the prediction of the effective mass model because no reflection with a zero y component is observed. For a small θ, the orientation of the vortex lattice is determined by pinning interactions between vortices and twin planes. Therefore, we postulate that this relation remains true for a larger θ, which leads to a quandary. The correlation length of the displacement field along the magnetic field direction, for θ = 50°, is resolution-limited and therefore at least ~2 μm. Hence, any bending of the vortex induced by the twin planes must be allowed to “heal” on a length scale shorter than the twin-plane spacing so that this bending does not cause a long-range displacement field reflecting the imperfect twin-plane periodicity. If, on the other hand, the vortex is assumed to be microscopically homogeneous, the pinning energy should not depend on the location of the intersection point between the vortex and the twin plane.

A length scale much shorter than the twin-plane spacing naturally arises in microscopic models of the vortex structure that also take the discreteness of the crystalline layer structure into account. In such models the vortex consists of “pancake” vortices in the ab plane separated by interplanar Josephson vortices. It has been argued (14) that the pinning forces experienced by the Josephson segments are reduced by a factor of (\( \epsilon(0/\epsilon) \)) with respect to the force experienced by pancake vortices. For YBa2Cu3O7, the in-plane coherence length is \( \xi = 15 \) Å and the interlayer spacing is \( d \sim 10 \) Å, so that
we can neglect the pinning force on the interlayer segments and concentrate on the pinning forces on the pancakes. For $e^r < 1$ and $\theta$ not too close to 90°, the projection of the lattice corresponding to the relation expressed in Eq. 1 onto the ab plane is an isotropic lattice with a lattice constant of 1.075 $\sqrt{3} \Lambda$. The pinning energy of the pancake vortices is maximized when one of the principal axes of this lattice is parallel to the “picket fence” pattern of twin boundaries. Viewed along the field direction, the reciprocal lattice vectors of the rotated lattice in the two twin-plane domains are

$$\mathbf{b}_1 = \frac{1}{\cos \theta} \left( \cos \theta \sin \theta \cos \phi \right)$$

$$\mathbf{b}_2 = \frac{1}{\cos \theta} \left( \cos \theta \sin \phi \cos \theta \right)$$

(2)

The high quality of our data allowed us to carry out a detailed quantitative analysis of the peak positions. The radial peak positions were obtained from fits to sector averages and were found to be in quantitative agreement with Eq. 2 for $\theta \leq 60^\circ$. Three-dimensional corrections apply for $\theta \geq 70^\circ$. To obtain the angular peak positions, we averaged the data radially in an elliptical annulus of appropriate eccentricity. Figure 4 shows the typical results of this procedure, together with the predictions from Eq. 2. Except for the unexplained asymmetry of a few reflections, the observed peak positions are in substantial agreement with Eq. 2. This agreement validates our simple model and necessitates an essentially two-dimensional pinning mechanism.

Finally, we focus on the diffraction pattern for $\theta = 90^\circ$ (Fig. 3P), which is inconsistent with Eq. 2. In fact, the anisotropic London model (Eq. 1) predicts the position of these reflections correctly. A reorientation of the vortex lattice into the unique orientation predicted by anisotropic London theory is expected for a large $\theta$ because the elastic energy for rotations away from this orientation increases markedly for a large $\theta$ (15). Fits to high-quality diffraction patterns for $B = 0.535$ T, $\theta = 77^\circ$, and neutron wavelengths ($\lambda$) of 6 and 10 $\AA$ yield a value of 0.0061 ± 0.0003 $\AA^{-1}$ for the radial peak position. The corresponding $e = 0.23 ± 0.05$ is within the errors consistent with the values extracted from Bitter decoration patterns (16, 17).

For a large $\theta$, the triangular vortex lattice is severely stretched in the direction perpendicular to both B and c and can be regarded as a collection of chains whose periodicities are locked. Anisotropic London theory predicts an attractive double well in the intervortex interaction along the chains for small fields, so that the vortices can penetrate as independent chains as the field is increased through the lower critical field $H_L$. Such a vortex chain state has been observed in low-field Bitter decoration in $YBa_2Cu_2O_y$ (17). Some workers (18) have used the same theory to predict the persistence of this vortex chain state to much larger fields, due to an exponential softening of the vortex-lattice shear modulus corresponding to translations of the chains in the chain direction. In $YBa_2Cu_3O_7$ for $B = 0.5$ T, the chains are predicted to decouple for $\theta \geq 80^\circ$ (18), thus giving rise to a diffraction pattern consisting of just two reflections. The data represented in Fig. 3P confirm this prediction. By translating the detector with respect to the beam to probe a wider momentum range and taking diffraction patterns for different values of $\theta$, we observed only broad and weak diffuse scattering around the remaining four reciprocal lattice vectors for fields of 0.1 and 0.5 T. The broadening of these Bragg peaks reflects the loss of long-range order in the direction perpendicular to the chains.

In contrast to observations in other anisotropic superconductors (2), but in agreement with observations in $YBa_2Cu_3O_y$ at low fields (17), we therefore conclude that the mean field anisotropic London theory (13, 18) provides an adequate description of the structure and orientation of the vortex lattice in this material. However, we have also shown that pinning to correlated microstructural defects can obliterate this intrinsic behavior and lead to unexpected changes in morphology and orientation of the vortex lattice as a function of $\theta$. It will be interesting to extend this investigation into a temperature and field range in which the melting of the flux-line lattice is expected to occur. For device applications, the strong response of the vortex lattice to the presence of twin planes, and the absence of any measurable influence of any other microstructural feature, makes the structural determination of twin planes a promising approach to enhance the flux-trapping properties of these materials.

**REFERENCES AND NOTES**

5. F. Dogan, unpublished data.
7. The neutron scattering experiments were conducted on the NS-7 small-angle neutron scattering spectrometer at the Cold Neutron Research Facility of the National Institute of Standards and Technology. The crystal was attached to the cold finger of a closed-cycle helium refrigerator that was then mounted in an electromagnet. Most of our data were taken at $B = 0.5$ T with neutrons of wavelength 6 $\AA$. After scattering from the sample, the neutrons were collected by an area detector $\pm 15^\circ$ behind the sample. We used the standard “horizontal field” scattering geometry in which the magnetic field is nearly parallel to the neutron beam (G. Lippmann, J. Schellen, W. Schmatz, Philos. Mag. 33, 475 (1976)). In this geometry the Bragg condition (with typical scattering angles of $2\theta = 0.5^\circ$) is strictly met only for those reflections for which the angle between the magnetic field and the beam is set to $\theta$. In practice, however, the nonzero width of the reflections in the $\phi$ direction, resulting from vortex bending or resolution effects such as the angular divergence of the incoming beam and crystal mosaicity, often allows the entire diffraction pattern to be taken while the beam is kept nominally parallel to B (that is, $\theta = 0$).
12. The critical angle we observe ($\theta_c \approx 30^\circ$ at $B = 45^\circ$) is substantially larger than the critical angles extracted from the transport measurements at comparable fields. Several corrections may apply (thermal wandering of the vortices around a twin plane, temperature dependence of the coherence...
Anatomy of the Photodissociation Region in the Orion Bar


Much of the interstellar gas resides in photodissociation regions whose chemistry and energy balance is controlled by the flux of far-ultraviolet radiation upon them. These photons can ionize and dissociate molecules and heat the gas through the photoelectric effect working on dust grains. These regions have been extensively modeled theoretically, but detailed observational studies are few. Mapping of the prominent Orion Bar photodissociation region at wavelengths corresponding to the carbon-hydrogen stretching mode of polycyclic aromatic hydrocarbons, the 1-0 S(1) line of molecular hydrogen, and the J = 1-0 rotational line of carbon monoxide allows the penetration of the far-ultraviolet radiation into the cloud to be traced. The results strongly support the theoretical models and show conclusively that the incident far-ultraviolet radiation field, not shocks as has sometimes been proposed, is responsible for the emission in the Orion Bar.

Photodissociation regions (PDRs), sometimes called photodissociated regions, are regions in which far-ultraviolet (FUV) photons with energies less than the hydrogen ionization limit dominate the energy balance of the gas.

M. M. Meixner, Radioastronomy Laboratory, University of California, Berkeley, CA 94720.
P. P. van der Werf, Max Planck Institut für extraterres- trische Physik, Giessenberga Strasse, D-8546 Garching bei München, Germany.
J. A. Tauber, Radioastronomy Laboratory, University of California, Berkeley, CA 94720, and ESA Astrophys- tics Division, ESTC, P.O. Box 299, NL-2200 AG Noordwijk, the Netherlands.
J. Stutzki, I. Physikalisches Institut, Universität Köln, Zülicherstrasse 77, W-5000 Köln 41, Germany.
D. Rank, Lick Observatory, University of California, Santa Cruz, CA 95060.

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