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X-RAY SEARCH FOR CDW IN SINGLE CRYSTAL $YBa_2Cu_3O_{7-\delta}$

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ABSTRACT

Recently, H. L. Edwards et al.[1] observed, in STM experiments at 20K, modulations in the CuO chain layer of cold-cleaved single crystals of $YBa_2Cu_3O_{7-\delta}$ which they interpreted as a possible charge density wave (CDW). Since X-ray scattering is an ideal tool for the study of static or dynamic lattice displacements, we performed a synchrotron X-ray study at beamline X14 at the NSLS of BNL on a high quality single crystal of $YBa_2Cu_3O_{7-\delta}$, which was mainly single domain with a spacially well localized volume fraction of other twin orientations of roughly 10%. Appropriate scattering configurations were chosen to enable observations of longitudinal or transverse CDWs with polarization either in the chain direction, ∥ <010> or ⊥ to it in <001>. The X-ray energy of 16keV allowed us to reach large momentum transfers to increase the sensitivity to lattice displacements. In none of our scans, which definitely covered the case of a 1-dimensional longitudinal CDW with propagation in the b direction as proposed by Edwards et al., did we find intensity other than the main Bragg peak(s) and the twin reflections. We therefore suspect that the STM finding may be a surface-induced phenomenon.

1. Introduction

Following the lead of Edwards et al.[1] who found strong evidence with the STM for a static (i.e. pinned) charge density wave (CDW) at the 001 surface of a single crystal of $YBa_2Cu_3O_{7-\delta}$, we have performed an extensive synchrotron X-ray search for this effect which, with X-rays, is invariably seen as a ("static") longitudinal modulation of the structure in which the resultant atomic displacements are parallel to the wave vector of the proposed CDW. Essentially we have been guided in our study by the findings of Edwards et al.[1] where they show real-space STM images of a cold-cleaved (001) surface of the $YBa_2Cu_3O_{7-\delta}$ crystal which reveal the Cu-O chain plane to be corrugated along the chains (the b-axis of the orthorhombic crystal) with a wavelength of ~1.3nm. These corrugations persist over several wavelengths but are only weakly correlated between chains. The

Fourier transform of a well-defined image therefore shows somewhat cigar-shaped and diffuse "satellites", sharper in the b*-direction but elongated normal to it (along a* and, by implication, c*). Through a number of tests they identified the observed modulation as a Fermi-surface-induced 1D CDW whose period was quite plausibly given by a known Fermi surface spanning length ($2k_F$) in the direction in question. The observed CDW's were perforce pinned both because they would otherwise not be seen in the STM and because observed oxygen vacancies could act as pinning centers.

The present study was thus made rather straightforward. For normal X-ray scattering the assignment of static vs. dynamic is not possible. However, the scattering is not off the CDW itself but invariably off the attendant displacement wave or mass density wave (MDW) resulting from the correlated core readjustments to the CDW. We therefore expect to measure satellite(s) about the average Bragg peaks which appear at $(2\pi)/\Lambda$ where Λ is the CDW wavelength. Actually, if the MDW is well-defined, even if it is sinusoidal, higher order satellites can be expected.[2] However, their absence is usually attributed to defects and variations in Λ. Without entering seriously into the scattering formalism we may note that for such (static or dynamic) displacive waves, the scattered intensity shows the following proportionality:[2]

$$I_{MDW} \propto |F|^2 \cdot e^{-2M} (\mathbf{Q} \cdot \varepsilon_{MDW})^2$$

where $|F|$ is the structure factor for the Bragg peak in question, 2M is a combined static and dynamic Debye-Waller factor, $\mathbf{Q}$ is the diffraction vector ($\hbar\mathbf{Q}$ is the momentum transfer in the experiment) and ε_{MDW} is the unit polarization of the MDW, usually longitudinal or transverse. When the propagation vector of the MDW, $\mathbf{q}_{MDW} \parallel \varepsilon_{MDW}$, the wave is longitudinal; when $\mathbf{q}_{MDW}$ is $\perp \varepsilon_{MDW}$, it is transverse.

In the present case we shall be looking at $\mathbf{q}$ vectors in a radial direction about the (080) position (i.e. longitudinal) where $\varepsilon_{MDW} \parallel \mathbf{q}_{MDW}$. For a transverse wave our principal experiments give $\varepsilon_{MDW} \perp \mathbf{q}_{MDW}$, and thus $\varepsilon_{MDW} \perp \mathbf{Q}$, and $\mathbf{Q} \cdot \varepsilon_{MDW}=0$! We thus measure only the longitudinal CDW contribution along the b-axis (b* reciprocal axis or k-direction using the conventional $hk\ell$ indices for our reciprocal lattice notation). We chose to measure at (080) because at this large value of Q the observed effect, $(\mathbf{Q} \cdot \varepsilon)^2$, will be much enhanced, if present, while the value of 2M is not so large as to cancel this advantage.

2. Experiment

Our study was done on a nominally single domain crystal of $YBa_2Cu_3O_{7-\delta}$ (0.5mm x 2.0mm x 0.06mm) from a batch with T_c's of ~91K, a transition width of <0.1K and an oxygen content $0 \leq \delta \leq 0.05$. The measured mosaic spread was less than 0.1°, although the wings of an azimuthal (transverse) scan through a Bragg peak will always show some sharp structure with synchrotron resolution. The crystal was mounted on a glass fiber in a He-filled, Be-walled, can in an evacuated displex cryostat Be chamber which was offsetmounted on a Huber 4-circle diffractometer on line X14 at the National Synchrotron Light Source (NSLS) at Brookhaven. The temperature was maintained at 23-24K. No analyzer crystal was used but a solid state detector was employed to remove fluorescence scattering (CuKα). The incident energy was 16keV (λ=0.7744Å) which is below the K-edge of Y (λ=0.7277Å) to leave a background relatively clean of parasitic scattering.

We show in Fig.1 a schematic of the twin structure to be expected in the reciprocal space of an orthorhombic crystal. The notations (1,2) and (3,4) refer to domains in which the a and b axes are reversed. From (1) to (4) or (2) to (3) we have twin related spots. As we explore the (080) reflection at lower intensity contours we can expect to see, not only weaker mosaic blocks, but the twinning and domain structure of Fig.1 even though our crystal consists <u>mainly</u> of one untwinned domain (~90%). As we shall see, however, the extensive structure is nowhere in evidence at the predicted positions of the CDW satellites (Λ=13Å, b=3.89Å): namely at a value of $\Delta k \simeq \pm 0.3$ from any 0k0 Bragg peak.

In Fig.2 we show a radial line scan through the major twin reflection at 080 where the central Bragg reflection is several orders of magnitude off scale and the twin reflection appears as a cut through its mosaic tail. Figures 3(a) and (b) show contour maps of the a*-b* plane covering two ranges: 3(a) shows contours running from 4.6×10^4 down to 10^3 counts. Figure 3(b) shows a much more diffuse (weaker) range covering 2×10^3 to 900 counts. At $\Delta k = \pm 0.3$, i.e. at k=8.3 and 7.7, there is no evidence in either plot for a diffuse structure parallel to the h-axis. The structure in Fig.3(a) results from a major twin domain centered on 080 with its twin arranged as in (2-3) of Fig.1. The second (weaker) pair (1-4) is shifted, as in Fig.1 to higher h by Δh=0.1. The split in k is only ~0.15. In other words, over an intensity range covering the weakest background scattering there is <u>no</u> evidence for the CDW (MDW) structure suggested by the results of Ref.1.

Figure 3(c) completes this picture with contour maps in the b*-c* plane about (080). Again there is the expected twin structure displaced in k by Δk~0.15 and showing extensive mosaic structure associated, again, with weak wings in this case along the c* direction (ℓ) which is also transverse to the radial <0k0> direction, but with no diffuse peaks ("cigars") along ℓ at k=8.3 or 7.7!

3. Conclusions

Based on our data to date, we conclude that the observations of Edwards et al. are related to a surface phenomenon and do not represent a bulk CDW. This result is, however, at variance with the recent report by Mook and co-workers at this conference in which their integrated neutron intensities along the suggested sheet of diffuse scattering at $\Delta k \simeq 0.3$ about (020) shows a peak. We have, at this time, no explanation for this discrepancy.

Acknowledgments

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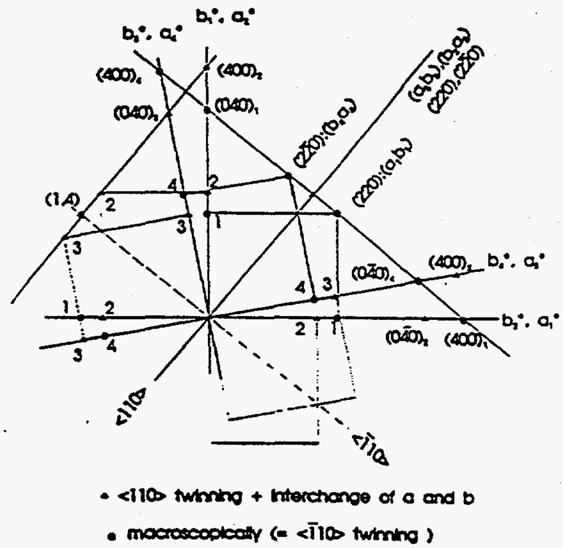


Fig. 1 Schematic reciprocal lattice for a twinned crystal with 2 domains.

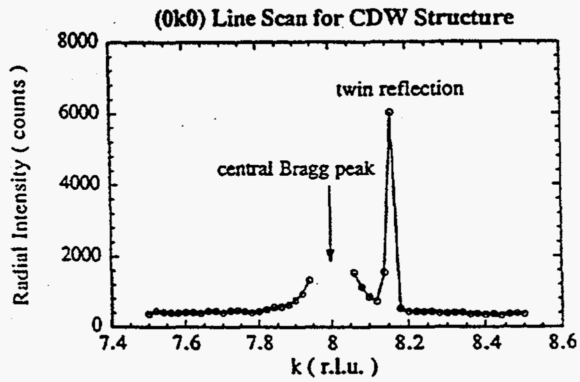
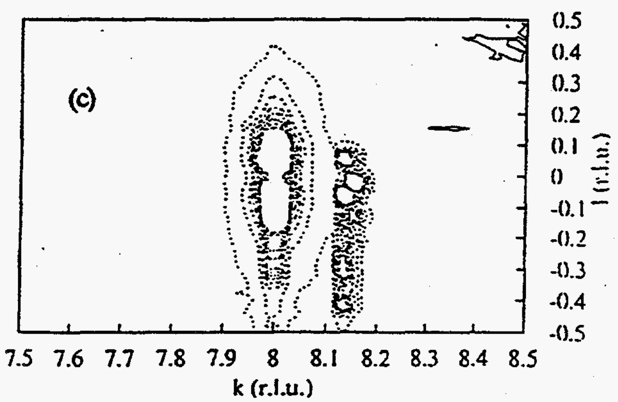


Fig. 2 Radial scan through major 080 reflection with no indication for peaks at 7.7 or 8.3.



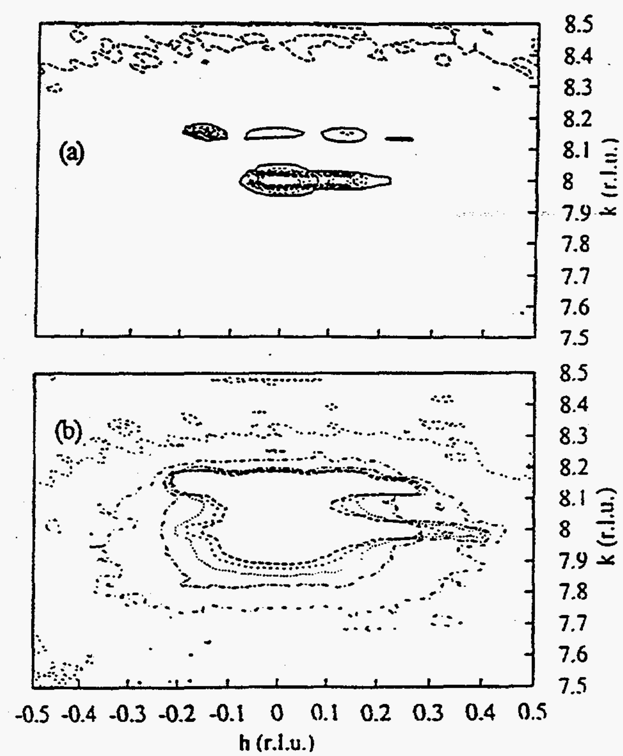


Fig. 3 (a) and (b): Contour maps in the a*-b* (hk0) plane: (a) contours run from $4x10^4$ to 10^3 counts; (b) runs from $2x10^3$ to 900; (c) contour map in b*-c* (0kℓ) plane. There is no evidence for CDW structure at $\Delta k = \pm 0.3$ (see text).